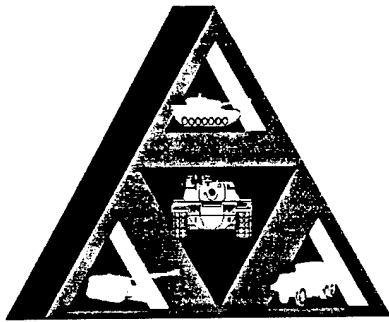# TARDEC

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Fuel Classification and Parameter Prediction Using GLC Analysis

April 1997

By   Donald Minus

U.S. Army Tank-automotive and Armaments Command
Research , Development and Engineering Center
Warren, Michigan 48397-5000

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Using a previously developed Gas Liquid Chromatography procedure for rapid characterization of fuel type and prediction of selected property values, different operators were used to develop the precision data for this methodology. The extremely low errors of prediction for both single versus multi operators attests to the universalness of this procedure.

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I   INTRODUCTION

Earlier reports detailed the use of Gas-Liquid Chromatograph (GLC) as an effective method for fuel type (i.e., gasoline, turbine fuel, and diesel fuel) classification and parameter prediction.[1,2] In these studies, more than two hundred fuel (200) samples were analyzed using several GLC columns and oven-parameter profile pairs. Predictions were made of the fuel's type using 10%, 50%, 90%, and final boiling point temperature distillation data, density at 25°C, and kinematic viscosity at 40°C. Using an HP-1 column and analyses times varying from 12 to 60 minutes, absolute errors of predictions were lower than 10 percent and correct fuel type classifications were higher than 95%.

Based on a previous report[2], a 15-minute analysis time was selected for further study. The 15-minute analysis time was chosen due to increase sample throughput and the fact that errors and classification percentages for the 15-minute analysis were comparable to the longer analyses.

II   INVESTIGATION

In the current report, four (4) summer-hire high school students performed the GLC analysis of selected fuel samples which were previously analyzed in the referenced reports.[1,2] Prediction models previously developed from the original data which was obtained by a single operator were then applied to the latest test results to determine the GLC methods' ability to accurately predict data on fuel samples run by different operators. Additionally, models were constructed from the latest multi-operators data and applied to the original single-operator data to determine the ability of models generated from the latest data at predicting the fuel parameters for the data from the single-operator analyses.

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[1] Superscript numbers refer to references at the end of the report.

III SAMPLES

In the current study, one hundred ten (110) samples were analyzed of which eighty-three (83) were diesel fuel Grade DF-2 conforming to Federal Specification VV-F-800D "Fuel Oil, Diesel"[3], eleven (11) were aviation gasoline (AV-GAS) conforming to American Society for Testing and Materials (ASTM) specification D910 "Standard Specification for Aviation Gasoline"[4], five (5) were JET A conforming to American Society for Testing and Materials (ASTM) D1655 "Standard Specification for Aviation Turbine Fuels"[5], five (5) were JP-4 samples and three (3) were JP-5 samples each conforming to Military Specification MIL-PRF-5624S "Turbine Fuel, Aviation, Grades JP-4, JP-5, and JP-5/JP-8 ST"[6], and three (3) were automotive gasoline (MOGAS) samples conforming to Military Specification MIL-G-3056F "Gasoline, Automotive, Combat".[7]

The fuel samples used in the study were obtained from three sources: the Fuels Branch, Fuels and Lubricants Division, Wright-Patterson Air Force Base (WPAFB), OH; Directorate of Aerospace Fuels, Detachment 13 (the Kelly AFB contingent at WPAFB); and the US Army TARDEC Fuels and Lubricants Research Facility (TFLRF) at SwRI, San Antonio, TX (formerly the Belvoir Fuels and Lubricants Research Facility (BFLRF). A list of the fuel samples used in the study is given in APPENDIX A and the specification test data for the fuel samples is given in the initial report.[1]

IV DESCRIPTION OF GLC TEST PARAMETERS

The Hewlett-Packard HP5890 Gas Chromatograph instrument (GC) was set to an initial temperature of 40°C, with a hold time of zero minutes, a program ramp rate of 25.0°C per minute, to a final temperature of 250°C, with a hold time of 6.6 minutes. A Flame Ionization Detector (FID) was used with a 10-meter megabore column, 0.53 cm inside diameter with a 2.65 μm film coat of methyl silicone (HP-1). The carrier gas was helium with a flow rate of 9.0 mL per minute. As defined in the earlier reports[1,2], the chromatograms were reduced to 20 data points by combining the chromatographic area in twenty time-segmented regions. The time constraints for the segmented-regions and the retention times for the unbranched normal alkanes under the forementioned conditions are given in Table 1.

TABLE 1: Time Constraint for Segmented Regions and Retention Time of Unbranched Normal Alkanes Under Test Conditions

Region	n-Alkane	Retention Time	Time Boundaries
1	C5	0.616 min	0.00 - 0.74 min
2	C6	0.871 min	0.74 - 1.09 min
3	C7	1.309 min	1.09 - 1.61 min
4	C8	1.909 min	1.61 - 2.25 min
5	C9	2.588 min	2.25 - 2.93 min
6	C10	3.265 min	2.93 - 3.59 min
7	C11	3.923 min	3.59 - 4.23 min
8	C12	4.544 min	4.23 - 4.83 min
9	C13	5.125 min	4.83 - 5.40 min
10	C14	5.673 min	5.40 - 5.93 min
11	C15	6.189 min	5.93 - 6.43 min
12	C16	6.679 min	6.43 - 6.91 min
13	C17	7.138 min	6.91 - 7.36 min
14	C18	7.588 min	7.36 - 7.80 min
15	C19	8.039 min	7.80 - 8.20 min
16	C20	8.360 min	8.20 - 8.67 min
17	C21	---------	8.67 - 9.22 min
18	C22	---------	9.22 - 9.76 min
19	C23	---------	9.76 - 10.31 min
20	C24	10.583 min	10.31 - 15.00 min

V   TEST PROCEDURE

Each operator injected one μL of the fuel sample into the GC and initiated data collection from the console. Once the run was completed, the operator transformed the data into the twenty time-segmented data points and entered the data into the correlation program spread sheet. A list of the twenty data points for each of the fuels is given in Appendix A. After determining the predicted values the data was statistically analyzed for accuracy of the prediction.

VI   RESULTS OF ANALYSIS

As in the earlier reports, the parameters that were considered were the 10%, 50%, 90%, and final boiling point (BP) distillation temperatures, the density measured at 25°C, and the kinematic viscosity measured at 40°C. To determine the universalness of the method, a three (3) data set was considered: one containing data that was previously developed performed by a single operator; one containing data from analyses performed by various operators, and one combined set containing data from both of the above-mentioned sets. Prediction models were developed from the data sets and were then applied to each of the data sets to determine the errors of predictions when using the models. The following are tables of the errors of predictions with explanations for each provided in the following paragraphs.

TABLE 2:   Errors of Prediction For Single-Operator Data Using Models Developed From Single-Operator Data

PARAMETER	AVG. ERR.	AVG. % ERR.	ABS. AVG. ERR.	ABS. AVG. % ERR.	MEASURED/ PREDICTED
10% BP TEMP (°K)	1.3	0.23	8.74	2.12	1.01
50 % BP TEMP (°K)	0.018	-0.12	5.99	1.41	1.00
90 % BP TEMP (°K)	-0.074	-0.076	9.19	1.88	1.00
FINAL BP TEMP (°K)	2.64	0.431	15.7	3	1.01
DEN @25°C(Kg/L)	0.00	0.01	0.01	0.647	1.00
VIS @40°C(cSt)	0.06	0.49	0.24	17.8	·1.06

AVG. ERR. is the average error for the parameter and is calculated by subtracting the predicted value of a sample parameter from the parameter value as measured by an independent accepted standard test method and taking the average for all samples in the data set.

(i.e., AVG. ERR. = $(\Sigma(Pm-Pc))/N$ where Pm is the parameter measured value, Pc is the parameter predicted value and N is the number of samples in the data set)

AVG. % ERR. is the average percent error for the parameter and is calculated by subtracting the predicted value of a sample parameter from the parameter value as measured by an independent accepted standard test method and dividing the resulting by the parameters measured value then multiplying by 100 and taking the average for all samples in the data set.

(i.e., AVG. % ERR. = $\Sigma(((Pm-Pc)/Pm)*100)/N$ where Pm is the parameter measured value, Pc is the parameter predicted value and N is the number of samples in the data set).

AVG. ABS. ERR. is the average absolute error for the parameter and is calculated by subtracting the predicted value of a sample parameter from the parameter value as measured by an independent accepted standard test method and taking the average of the absolute value of the number for all samples in the data set.

(i.e., AVG. ABS. ERR. = $(\Sigma(|Pm-Pc|))/N$ where Pm is the parameter measured value, Pc is the parameter predicted value and N is the number of samples in the data set)

AVG. ABS. % ERR. is the average absolute percent error for the parameter and is calculated by subtracting the predicted value of a sample parameter from the parameter value as measured by an independent accepted standard test method and dividing the resulting by the parameters measured value then multiplying by 100 and taking the average for all samples in the data set.

(i.e., AVG. ABS. % ERR. = $\Sigma(((|Pm-Pc|)/Pm)*100)/N$ where Pm is the parameter measured value, Pc is the parameter predicted value and N is the number of samples in the data set).

Measured/Predicted is the average of the parameter's measured value divided by its predicted value and is calculated by dividing the parameter's measured value by its predicted value and taking the average of all samples in the data set.

(i.e., Measured/Predicted = $(\Sigma(Pm/Pc))/N$ where Pm is the parameter measured value, Pc is the parameter predicted value and N is the number of samples in the data set)

TABLE 3:   Errors of Prediction for Multi-operator Data Using Models Developed from Multi-operator Data

PARAMETER	AVG. ERR.	AVG. % ERR.	ABS. AVG. ERR.	ABS. AVG.% ERR.	MEASURED/ PREDICTED
10% BP TEMP (°K)	2.65	0.20	12.4	2.88	1.00
50% BP TEMP (°K)	1.96	0.09	10.9	2.28	1.00
90% BP TEMP (°K)	6.43	0.82	16.6	3.15	1.01
FINAL BP TEMP (°K)	5.96	0.67	20.9	3.78	1.01
DEN @25°C(Kg/L)	0.00	0.20	0.01	0.97	1.00
VIS @40°C (cSt)	-0.03	-5.07	0.21	12.3	0.98

TABLE 4:   Errors of Prediction for Single-operator and Multi-Operator Data Using Models Developed from Single-Operator and Multi-operator Data

PARAMETER	AVG. ERR.	AVG. % ERR.	ABS. AVG. ERR.	ABS. AVG. % ERR.	MEASURED/ PREDICTED
10% BP TEMP (°K)	1.15	0.21	10.4	2.61	1.04
50 % BP TEMP (°K)	0.00	-0.11	7.27	1.61	1.00
90 % BP TEMP (°K)	0.00	-0.11	11.8	2.38	1.00
FINAL BP TEMP (°K)	-0.11	-0.24	17.7	3.35	1.00
DEN @25°C (Kg/L)	0.00	0.07	0.01	0.82	1.00
VIS @40°C (cSt)	-0.03	-4.48	0.18	12.0	0.98

TABLE 5:   Errors of Prediction for Single-operator Data Using Models Developed from
Multi-operator Data

PARAMETER	AVG. ERR.	AVG. % ERR.	ABS. AVG. ERR.	ABS. AVG. % ERR.	MEASURED/ PREDICTED
10% BP TEMP (°K)	8.23	1.71	14.9	3.59	1.02
50 % BP TEMP (°K)	4.53	0.72	12.2	2.75	1.01
90 % BP TEMP (°K)	-5.27	-1.25	13.9	2.92	0.99
FINAL BP TEMP (°K)	-5.01	-1.21	20.5	3.99	0.99
DEN @25°C (Kg/L)	-0.001	-0.156	0.007	0.907	1.00
VIS @40°C (cSt)	-0.002	-0.340	0.009	1.09	1.00

TABLE 6:   Errors of Prediction for Multi-operator Data Using Models Developed from
Single-operator Data

PARAMETER	AVG. ERR.	AVG. % ERR.	ABS. AVG. ERR.	ABS. AVG. % ERR.	MEASURED/ PREDICTED
10% BP TEMP (°K)	1.57	0.45	6.63	1.51	1.00
50% BP TEMP (°K)	-0.34	0.04	6.04	1.24	1.00
90% BP TEMP (°K)	-1.18	-0.01	9.68	1.88	1.00
FIN. BP TEMP (°K)	-0.76	-0.026	9.72	1.75	1.00
DEN @25°C (Kg/L)	-0.002	-0.26	0.005	0.576	0.99
VIS @40°C (cSt)	-0.02	-0.008	0.124	7.49	1.01

VII SUPPORTING DATA

Appendix A provides the Tables of Peak Density for the twenty (20) Segmented Regions. Appendix B gives the Numerical Formulas for Calculating Predicted Parameters' Values Using the Percent Peak Area in Segmented Regions. Appendix C provides Plots of Measured Versus Predicted Parameters using Models Generated using Data from GLC Traces of the Summer-Hire Students Combined with Previously-Ran Single Operator Data. Appendix D gives Plots of Measured Versus Predicted Parameters using Models Generated using Data from GLC Traces of the Previously-Ran Single Operator Data. Appendix E provides Plots of Measured Versus Predicted Parameters using Models Generated using Data from GLC Traces of the Summer-Hire Students.

VIII CONCLUSIONS

The low errors of predictions for both the single-operator and multi-operator data sets details the ability of the GLC method to accurately predict parameter values data independent of the operator.

The final phase of laboratory verification of the method should include various operators in various laboratory using equipment other than the GLC used in the initial study. This would validate the universalness of the method independent of the operator and the GLC system.

IX REFERENCES

1. Minus, D. K., "Fuel-Type Classification and Parameters Prediction by Gas Liquid Chromatography Analysis", TARDEC Technical Report # 13641, February, 1995, U. S. Army Tank-Automotive Research, Development and Engineering Center, Warren, MI.

2. Minus, D. K., "Statistical Analysis of Parameter Prediction of Various Military Fuel Samples..." TARDEC Technical Report #13647, February 1996, U. S. Army Tank-Automotive Research, Development and Engineering Center, Warren, Michigan MI.

3. ASTM D1655 "Standard Specification for Aviation Turbine Fuels". American Society For Testing And Materials, 1916 Race Street, Philadelphia PA.

4. Military Specification MIL-PRF-5624S, "Turbine Fuel, Aviation, Grades JP-4, JP-5, and JP-5/JP-8ST", 22 November 1996.

5. ASTM D910 "Standard Specification for Aviation Gasolines." American Society For Testing and Materials, 1916 Race Street, Philadelphia PA.

6. Military Specification MIL-T-83133D, "Turbine Fuels, Aviation, Kerosene Types, NATO F-34 (JP-8) and NATO F-35", January 1992.

7. Military Specification MIL-G-3056F, "Gasoline, Automotive, Combat", November 1991.

8. Federal Specification VV-F-800D, "Fuel Oil, Diesel", October 1987. (Note: this has been canceled and replaced with Commercial Item Description CID A-A-52557 Fuel Oil, Diesel; for Posts, Camps and Station).

X ACKNOWLEDGMENTS

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Appendix A
Tables of Peak Density in Segmented Regions

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SAMPLE	338SH1	444CF1	449MF1	539TS1	551MF1	586SH1	609DM1
Region 1	0.1900	0.0160	0.6900	0.5700	0.1800	1.4300	0.1100
Region 2	8.4500	0.0960	9.6100	9.9000	14.3900	6.5000	3.8800
Region 3	33.6200	0.5300	16.3700	30.7900	40.2600	21.2000	53.4800
Region 4	48.3400	1.3500	18.4000	46.1000	35.8000	11.7400	42.5300
Region 5	3.9600	4.3800	18.3000	3.4800	3.6500	11.2700	0.0000
Region 6	2.2300	12.1800	17.0200	1.9000	3.0320	10.9400	0.0000
Region 7	1.4800	20.0400	10.6500	2.1600	1.4400	8.1200	0.0000
Region 8	0.8000	18.9400	5.7500	1.8200	0.6000	8.7000	0.0000
Region 9	0.3600	16.3000	1.8700	1.3200	0.2000	8.2500	0.0000
Region 10	0.1900	10.8700	0.5100	0.9200	0.1600	5.9600	0.0000
Region 11	0.1100	9.6700	0.1900	0.5900	0.0960	4.5000	0.0000
Region 12	0.0600	4.3700	0.1500	0.2700	0.0470	0.9700	0.0000
Region 13	0.0555	1.1300	0.1200	0.1200	0.0000	0.2600	0.0000
Region 14	0.0240	0.0890	0.0700	0.0220	0.0460	0.0270	0.0000
Region 15	0.0210	0.0290	0.0380	0.0150	0.0000	0.0270	0.0000
Region 16	0.0310	0.0140	0.0470	0.0170	0.0380	0.0140	0.0000
Region 17	0.0330	0.0240	0.0240	0.0000	0.0680	0.0160	0.0000
Region 18	0.0450	0.0063	0.0410	0.0130	0.0000	0.0160	0.0000
Region 19	0.0000	0.0100	0.0310	0.0000	0.0000	0.0110	0.0000
Region 20	0.0000	0.5160	0.1200	0.0000	0.0000	0.0490	0.0000

SAMPLE	610SH1	625SH1	638GR1	638H1	640DM1	665DM1	665SH1
Region 1	0.1700	1.6200	3.3800	3.3900	0.6800	0.0100	0.0100
Region 2	0.7010	10.2000	11.5800	11.8700	9.2100	0.0400	0.0500
Region 3	29.7900	16.2500	21.3900	19.9700	25.6700	0.3200	0.4000
Region 4	55.6500	10.6300	19.7700	22.0000	12.0700	0.8100	0.8800
Region 5	4.0500	10.8600	18.5000	18.9500	9.5600	2.5100	2.5300
Region 6	1.4700	11.5000	16.5000	14.6800	10.0400	6.6200	6.3300
Region 7	1.1200	9.3600	5.0400	6.3100	8.7300	18.1500	18.0300
Region 8	0.4000	9.1400	1.7800	1.5000	8.2200	20.1600	23.1700
Region 9	0.1440	9.3500	0.8400	0.6130	7.2400	20.4600	18.5000
Region 10	0.0770	6.8300	0.4400	0.2200	4.8000	18.2400	14.4600
Region 11	0.0610	3.1900	0.3000	0.1500	2.7300	9.4400	12.3500
Region 12	0.0310	0.8400	0.1600	0.0870	0.9200	2.5300	2.9600
Region 13	0.0150	0.1660	0.0790	0.0550	0.3300	0.5400	0.2600
Region 14	0.0100	0.0190	0.0500	0.0320	0.0500	0.0300	0.0320
Region 15	0.0093	0.0110	0.0380	0.0230	0.0200	0.0100	0.0100
Region 16	0.0000	0.0100	0.0330	0.0310	0.0200	0.0100	0.0100
Region 17	0.0000	0.0110	0.0190	0.0280	0.0200	0.0200	0.0000
Region 18	0.0000	0.0100	0.0130	0.0110	0.0200	0.0100	0.0000
Region 19	0.0000	0.0076	0.0050	0.0040	0.0200	0.0100	0.0100
Region 20	0.0000	0.0000	0.0780	0.0700	0.0000	0.0600	0.0000

SAMPLE	653SH1	640SH1	644SH1	668GR1	668SH1	609DM1	21802DM1
Region 1	4.1000	2.8900	0.0100	0.0000	0.0000	0.1100	0.0100
Region 2	9.8100	7.6200	3.7300	0.0000	0.0400	3.8800	0.0200
Region 3	12.2300	24.8000	23.1000	0.0300	0.1400	53.4800	0.1200
Region 4	7.2900	11.6900	44.5600	0.2400	0.2400	42.5300	0.3500
Region 5	8.9600	9.4200	9.7800	2.0400	1.8400	0.0000	1.1300
Region 6	15.4000	10.4300	5.0100	9.5900	9.0600	0.0000	4.2900
Region 7	11.5000	8.6600	3.2700	20.1800	20.2200	0.0000	10.1800
Region 8	12.5000	8.2300	3.1700	24.7600	22.8100	0.0000	11.7200
Region 9	10.2100	7.2400	2.7200	19.9600	18.8300	0.0000	15.5500
Region 10	5.3600	4.3400	2.2500	11.6700	13.1100	0.0000	12.4000
Region 11	1.8400	3.1500	1.5300	5.8400	7.2400	0.0000	14.3000
Region 12	0.5300	1.0300	0.4800	2.7900	3.2500	0.0000	7.0800
Region 13	0.1400	0.3500	0.1500	1.5900	1.5800	0.0000	4.1100
Region 14	0.0200	0.0900	0.0800	0.8500	0.8600	0.0000	6.4400
Region 15	0.0100	0.0200	0.0600	0.1800	0.4000	0.0000	3.0000
Region 16	0.0200	0.0100	0.0300	0.0800	0.1700	0.0000	2.9400
Region 17	0.0200	0.0200	0.0300	0.0400	0.0400	0.0000	2.8600
Region 18	0.0200	0.0100	0.0300	0.0300	0.0300	0.0000	1.4800
Region 19	0.0000	0.0100	0.0200	0.0300	0.0200	0.0000	0.9900
Region 20	0.0000	0.0000	0.0000	0.0800	0.0700	0.0000	1.0100

SAMPLE	21819DM1	20909DM1	20814DM1	20830DM1	20823DM1	22687DM1	22673DM1
Region 1	0.0100	0.0100	0.0000	0.0000	0.0000	0.0000	0.0000
Region 2	0.0000	0.0100	0.0000	0.0000	0.0000	0.0000	0.0000
Region 3	0.0300	0.0400	0.0100	0.0100	0.0100	0.0300	0.0100
Region 4	0.1000	0.2300	0.0900	0.0800	0.0500	0.1300	0.0500
Region 5	0.6200	0.8200	0.4900	0.2400	0.2400	0.5000	0.3000
Region 6	2.9300	2.3700	2.0600	0.9200	0.9500	1.6800	1.9900
Region 7	5.4700	3.6800	5.7000	2.9200	3.3800	3.4500	5.9100
Region 8	8.4500	4.3700	6.8300	3.6800	4.7000	5.2300	10.3200
Region 9	10.2400	8.3200	9.9100	5.3900	5.0200	8.8000	11.2900
Region 10	13.6700	9.8500	9.4800	7.2300	9.2400	12.9300	14.4400
Region 11	14.8300	11.7300	7.2900	14.1000	11.7000	14.4100	14.1700
Region 12	11.2200	11.7700	11.7600	14.1000	13.1300	14.3600	10.2400
Region 13	8.5900	10.9500	10.8700	13.1900	12.5000	9.8800	7.3600
Region 14	6.9100	9.7800	11.0200	12.6500	11.3000	8.1000	6.4500
Region 15	5.6900	7.5000	8.6000	9.9200	9.4800	6.7600	5.3700
Region 16	4.3600	7.8300	7.8900	8.0500	7.7400	6.0200	4.8200
Region 17	3.3600	5.4700	3.7100	5.8600	6.5500	5.3700	4.0900
Region 18	1.6500	1.6700	2.2900	0.6900	1.9900	1.3200	1.3600
Region 19	0.6500	1.7000	1.1000	0.1800	0.7900	0.0800	0.6300
Region 20	1.2100	1.9000	0.8900	0.7700	1.2300	0.9500	1.1800

SAMPLE	22709DM1	22809DM1	22613DM1	22748DM1	22622DM1	22610DM1	22641DM1
Region 1	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Region 2	0.0300	0.0000	0.0000	0.0000	0.0000	0.0100	0.0100
Region 3	0.2800	0.0200	0.0200	0.0200	0.0300	0.0300	0.0500
Region 4	0.3800	0.0500	0.1300	0.1200	0.1300	0.2300	0.2800
Region 5	0.3300	0.3200	0.4900	0.5000	0.8800	1.4300	0.5100
Region 6	1.5500	1.7200	1.2300	1.2200	2.3200	3.5700	1.6200
Region 7	3.3600	3.7300	2.7300	3.7300	5.8100	8.6100	3.5600
Region 8	7.1200	6.7100	4.6400	4.6000	6.5400	8.1400	5.6300
Region 9	9.6300	9.9100	8.6400	8.6000	11.2000	11.9800	8.4200
Region 10	13.6100	13.3800	17.0900	17.1000	17.3800	13.6300	12.9500
Region 11	15.0600	15.9300	13.9200	14.0000	11.2400	12.7500	11.5300
Region 12	12.5400	13.0900	12.2000	12.2000	10.6100	8.1200	12.7600
Region 13	9.1600	8.6600	12.0000	12.0000	10.1600	9.2100	13.0100
Region 14	7.8800	13.2800	8.7900	8.8000	8.2100	6.8300	10.2400
Region 15	6.7000	5.9100	7.2600	7.2000	6.5000	5.7100	7.7400
Region 16	3.6400	2.5500	6.0000	6.0000	5.1000	4.9800	6.5800
Region 17	5.2500	3.0300	2.6800	2.7000	2.1600	2.4800	2.7800
Region 18	1.7500	0.8500	1.3800	1.4000	1.1600	1.4600	1.5400
Region 19	0.7600	0.3500	0.2200	0.2000	0.1600	0.1900	0.2100
Region 20	0.9800	0.4900	0.5900	0.6000	0.4100	0.6600	0.5600

SAMPLE	22625DM1	22651DM1	374DM1	560MF1	22645DM1	22616DM1	22607DM1
Region 1	0.0000	0.0000	0.0000	0.0200	0.0000	0.0000	0.0000
Region 2	0.0100	0.0000	0.0100	0.1600	0.0000	0.0000	0.0000
Region 3	0.0400	0.0200	0.1100	0.8300	0.0200	0.0200	0.0200
Region 4	0.2600	0.1300	0.6400	1.6400	0.1500	0.1500	0.1300
Region 5	0.6600	0.9200	2.8300	4.2400	0.4400	0.4400	0.4500
Region 6	2.9600	2.3600	11.0500	10.3200	1.7400	1.7300	1.2600
Region 7	7.1000	6.5400	21.4100	18.3700	4.1200	4.1100	2.9900
Region 8	7.4300	7.3700	21.9600	17.3500	6.6800	5.2500	3.4800
Region 9	12.8900	13.4400	19.5200	17.6700	8.9200	9.9400	5.6400
Region 10	14.8600	15.0100	13.2600	15.1500	13.4700	13.3300	8.9800
Region 11	10.4300	10.4300	6.7800	7.9600	10.4800	10.5200	9.4000
Region 12	9.7600	9.4400	1.5100	4.4700	14.1600	13.7300	9.3300
Region 13	9.0300	8.8800	0.6100	1.4200	13.3700	10.1300	13.2900
Region 14	7.4200	7.2900	0.2100	0.1600	8.5400	10.9200	17.5800
Region 15	6.3500	6.4100	0.0030	0.1100	7.4600	9.6100	11.3800
Region 16	5.2900	5.7000	0.0100	0.0200	5.8500	5.6500	9.6300
Region 17	2.7600	3.0500	0.0200	0.0100	3.9000	3.8200	5.7900
Region 18	1.5700	1.8100	0.0100	0.0200	0.3500	0.3300	0.3400
Region 19	0.1900	0.2000	0.0000	0.0200	0.0900	0.0690	0.0600
Region 20	0.9800	1.0000	0.0400	0.0500	0.2600	0.2570	0.2300

SAMPLE	22648DM1	22604DM1	551DM2	22619DM1	22642DM1	22568DM1	22592DM1
Region 1	0.0100	0.0100	1.4100	0.0000	0.0000	0.0000	0.0000
Region 2	0.0000	0.0900	11.0700	0.0100	0.0000	0.0000	0.0000
Region 3	0.0200	0.2600	53.9100	0.0900	0.0300	0.0200	0.0100
Region 4	0.1300	0.0600	29.2400	0.1100	0.1100	0.1700	0.0800
Region 5	0.4500	0.5000	1.3500	0.6000	0.5300	0.5300	0.3700
Region 6	1.2600	1.6300	1.8100	3.2300	2.4900	2.6100	1.5700
Region 7	2.9900	6.2400	0.6100	7.6000	6.3200	5.8300	5.3000
Region 8	3.4800	10.6200	0.1200	10.0400	6.5700	6.4400	6.7700
Region 9	5.6400	13.7300	0.1500	14.6800	10.4600	10.5600	12.6600
Region 10	8.9800	14.7800	0.0800	13.6400	12.8300	14.7700	15.4500
Region 11	9.4000	10.1400	0.0600	11.6500	12.6000	11.2400	13.9300
Region 12	9.3300	9.3400	0.0500	8.1700	12.2000	12.5000	13.0500
Region 13	13.2900	8.9200	0.0500	7.7900	9.5100	9.7800	9.0000
Region 14	17.5800	7.5200	0.0400	6.2200	8.6300	8.0700	6.8500
Region 15	11.3800	6.6100	0.0200	5.6300	7.2400	6.8900	5.8400
Region 16	9.6300	5.5600	0.0100	4.4700	5.7000	5.7000	4.7100
Region 17	5.7900	2.4600	0.0200	3.8200	2.6100	2.7000	2.2100
Region 18	0.3400	1.1800	0.0100	1.2200	1.3100	1.3800	1.1600
Region 19	0.0600	0.1200	0.0000	0.0800	0.1500	0.1700	0.1500
Region 20	0.2300	0.2600	0.0000	0.9900	0.7200	0.6300	0.8800

SAMPLE	22577DM1	22580DM1	22601DM1	22571DM1	22583DM1	22574DM1	22561DM1
Region 1	0.0000	0.0000	0.0000	0.0100	0.0000	0.0100	0.0000
Region 2	0.0000	0.0000	0.0100	0.0000	0.0000	0.0100	0.0000
Region 3	0.0100	0.0100	0.0300	0.0300	0.0500	0.0300	0.0300
Region 4	0.0900	0.0800	0.1800	0.1900	0.3700	0.1300	0.1600
Region 5	0.5100	0.7000	0.6300	0.4900	1.3900	0.9900	0.8900
Region 6	2.2200	3.6200	2.1100	2.1200	4.5700	2.5500	3.9200
Region 7	9.2400	10.0900	5.4400	5.8500	6.1600	6.9200	8.1600
Region 8	10.4800	8.2800	6.7000	7.8000	8.9600	6.8100	10.6100
Region 9	17.7700	14.3900	11.8800	11.4000	9.9600	11.5000	14.0100
Region 10	13.1100	15.7300	13.4500	12.9500	16.0400	14.3300	16.3300
Region 11	15.0300	15.0900	13.1000	13.4000	14.6700	10.5200	13.1500
Region 12	12.0300	12.0100	12.3600	12.6900	11.2900	10.3100	7.1900
Region 13	6.4400	6.9100	9.7100	8.9700	8.9900	9.8100	7.3600
Region 14	4.6500	4.5600	7.4900	7.3900	6.2000	7.6400	5.2500
Region 15	3.5100	3.3400	6.0900	6.3900	4.9900	6.5700	4.3200
Region 16	2.7700	2.8000	5.1000	4.9000	3.6500	5.5500	3.5300
Region 17	1.1400	1.1700	3.7700	3.9900	1.2600	4.3000	2.7600
Region 18	0.4900	0.0640	1.2600	0.5000	0.6700	1.3700	1.0400
Region 19	0.1000	0.0800	0.1300	0.1000	0.2800	0.1400	0.2800
Region 20	0.4200	0.4900	0.5600	0.8800	0.5000	0.5000	1.0100

SAMPLE	22564DM1	22595DM1	22598DM1	22586DM1	22419DM1	22411DM1	444DM1
Region 1	0.0000	0.0000	0.0100	0.0000	0.0000	0.0000	0.0200
Region 2	0.0000	0.0000	0.0100	0.0000	0.0300	0.0000	0.1100
Region 3	0.0200	0.0200	0.0200	0.0200	0.0900	0.0100	0.4300
Region 4	0.1700	0.1100	0.1800	0.1100	0.2700	0.1700	1.3700
Region 5	0.4700	0.5400	0.7400	0.5400	0.6500	1.6900	4.7100
Region 6	2.1600	2.1000	2.3400	2.0600	1.7200	11.4700	13.0600
Region 7	4.7000	4.6300	5.3500	4.6300	3.4800	21.8900	22.1900
Region 8	6.6900	7.0000	8.3900	7.0000	5.6200	25.7600	15.0900
Region 9	11.1800	14.7100	11.2000	14.7100	9.3700	22.3600	11.1900
Region 10	14.0300	15.4200	13.0100	15.4200	16.3200	10.6900	14.2700
Region 11	12.4200	10.5800	13.0100	10.5800	17.4400	2.7000	12.0300
Region 12	13.2600	13.8800	12.5100	13.8800	9.0800	1.0700	4.0200
Region 13	9.0200	11.2700	8.5600	11.2700	7.9900	0.6000	1.1000
Region 14	9.5700	7.5600	9.9100	7.5600	6.3300	0.3800	0.0900
Region 15	6.5200	6.0400	7.7000	6.0400	5.2700	0.2700	0.1000
Region 16	4.5400	3.3700	3.8700	3.3700	5.0700	0.3100	0.0500
Region 17	4.2100	2.1600	2.6900	2.1600	4.8600	0.1700	0.0500
Region 18	0.5500	0.3400	0.2500	0.3400	1.9500	0.1400	0.0200
Region 19	0.0800	0.0500	0.0500	0.0500	0.9700	0.0800	0.0100
Region 20	0.4000	0.2800	0.2000	0.2800	3.5000	0.2100	0.0900

SAMPLE	609SH1	610SH1	638DM1	20821DM1	20824DM1	20827DM1	20837DM1
Region 1	0.0200	0.1300	2.6200	0.0000	0.0000	0.0000	0.0000
Region 2	2.2600	2.9300	10.6500	0.0000	0.0000	0.0000	0.0100
Region 3	29.8600	33.0000	22.0900	0.0100	0.0100	0.0200	0.0400
Region 4	49.6900	55.5000	20.9800	0.0500	0.0400	0.1300	0.1300
Region 5	9.0600	4.9900	15.7500	0.2800	0.3000	0.5600	0.5100
Region 6	3.1400	1.2200	16.5900	1.4900	1.6800	1.9600	1.2100
Region 7	5.0500	1.1900	6.2000	3.4800	4.4000	4.5200	3.5000
Region 8	0.3700	0.0000	2.4900	6.3400	7.6400	6.4900	4.5500
Region 9	0.1700	0.2200	1.1900	9.9800	13.0400	9.6100	8.8100
Region 10	0.0900	0.1600	0.4800	13.3000	13.9500	11.9400	13.1400
Region 11	0.0700	0.1000	0.3500	14.0300	9.5300	12.2900	14.7200
Region 12	0.0600	0.0600	0.2100	13.2700	13.4800	12.2400	13.5800
Region 13	0.0500	0.0100	0.1200	8.1900	11.2600	11.6000	10.2600
Region 14	0.0400	0.0000	0.0200	10.4200	9.2900	10.3500	8.6900
Region 15	0.0300	0.0000	0.0600	7.5100	7.3400	7.1600	7.2100
Region 16	0.0300	0.0000	0.3200	5.0400	4.1400	5.1400	6.5400
Region 17	0.0200	0.0000	0.0300	4.1200	3.1900	4.0500	5.3600
Region 18	0.0200	0.0000	0.0200	1.1700	0.7100	0.1000	1.7500
Region 19	0.0100	0.0000	0.0200	0.0000	0.0000	1.2200	0.0000
Region 20	0.0000	0.0000	0.0700	0.9600	0.0000	0.0000	0.0000

SAMPLE	20837DM2	20838DM1	20839DM1	21748DM2	21792DM1	21794DM2	21796DM1
Region 1	0.0000	0.0000	0.0100	0.0000	0.0300	0.0100	0.0000
Region 2	0.0000	0.0000	0.0000	0.0000	0.0300	0.0100	0.0000
Region 3	0.0200	0.0100	0.0000	0.0300	0.1000	0.1000	0.0500
Region 4	0.0700	0.0600	0.0300	0.1900	0.3700	0.3500	0.2200
Region 5	0.2200	0.3300	0.2100	1.0800	1.4700	1.2100	0.7800
Region 6	0.7400	1.2400	1.2400	4.0100	4.7800	3.9600	2.7000
Region 7	2.1500	3.2300	3.5000	8.3800	7.7900	7.0700	5.1300
Region 8	3.0500	5.5400	4.8100	11.1700	9.0800	9.1800	7.2300
Region 9	5.8300	8.7300	5.3000	16.8600	12.4400	13.0900	10.6800
Region 10	7.3200	12.2800	11.1000	13.7700	13.5000	13.7000	12.1800
Region 11	12.6800	15.0400	11.3000	13.1300	11.1200	12.7800	12.5800
Region 12	12.9800	15.7000	11.6400	7.4100	11.3300	10.5000	12.1200
Region 13	12.6900	13.3000	12.1500	6.5300	6.7400	9.6800	11.2200
Region 14	11.9400	7.7100	11.4400	4.7900	7.3600	6.4200	9.4700
Region 15	9.4400	7.4000	10.0300	4.2600	5.8200	5.0700	6.4100
Region 16	7.7700	4.8200	7.8300	3.5900	3.5800	2.9700	4.3800
Region 17	6.7400	3.2400	6.1300	3.0500	2.7100	2.4200	3.4000
Region 18	0.5000	0.7900	1.6600	0.9700	0.8700	0.7600	0.5800
Region 19	2.4200	0.5700	0.5300	0.0500	0.3500	0.0200	0.8700
Region 20	3.4400	0.0000	1.0800	0.6900	0.5500	0.7000	0.0000

SAMPLE	21800DM1	21807DM1	21809DM1	21815DM2	21821DM1	21833DM1	21837DM1
Region 1	0.0100	0.0300	0.0100	0.0900	0.0100	0.0300	0.0100
Region 2	0.0000	0.0200	0.0100	0.0400	0.0100	0.0200	0.0000
Region 3	0.0500	0.0900	0.0400	0.1900	0.0400	0.0800	0.0100
Region 4	0.2600	0.3600	0.2200	0.5100	0.2100	0.2400	0.1000
Region 5	0.9800	1.5200	1.1700	1.6400	0.8200	0.6100	0.7100
Region 6	2.4300	5.4100	4.2200	4.1500	2.6200	1.7200	2.9100
Region 7	4.7300	10.1200	6.9300	6.6400	4.3300	3.6000	8.3800
Region 8	7.8400	12.1600	8.8700	8.1000	5.6500	5.8800	14.2600
Region 9	15.1400	15.1700	12.9500	11.7900	8.0300	9.2800	20.5100
Region 10	13.8400	14.3900	12.4900	10.9600	9.8200	13.2000	15.4900
Region 11	8.6400	12.1400	7.7700	11.3000	11.1000	14.6900	12.4600
Region 12	12.4200	6.5700	10.7100	7.5600	10.8200	14.0300	5.7400
Region 13	11.6000	5.6600	10.1700	7.6900	11.5200	10.1300	5.3400
Region 14	9.5700	6.5800	9.6000	8.8400	10.3800	10.8000	4.7100
Region 15	6.3800	4.2000	6.4800	7.2000	7.9100	7.5900	4.0000
Region 16	3.2800	2.8700	4.4100	5.1100	5.8300	4.3800	3.2700
Region 17	2.1800	2.2400	3.3100	4.4400	4.8500	2.9900	1.3300
Region 18	0.3800	0.2800	0.1900	1.6200	2.7700	0.3200	0.5400
Region 19	0.0400	0.0300	0.0000	0.0000	1.5300	0.0800	0.0500
Region 20	0.2400	0.1600	0.4200	2.1300	1.7300	0.3300	0.1600

SAMPLE	21839DM1	21841DM1	21844DM1	21862DM1	21883DM1	21885DM1	21887DM1
Region 1	0.0100	0.0000	0.0000	0.0000	0.0100	0.0100	0.0000
Region 2	0.0100	0.0000	0.0000	0.0000	0.0500	0.0700	0.0000
Region 3	0.0700	0.0100	0.0100	0.0000	0.2600	0.2400	0.0100
Region 4	0.2700	0.0500	1.0400	0.1000	1.2400	1.2000	0.0500
Region 5	0.8200	0.4100	6.3000	1.6400	3.9800	4.6000	0.3400
Region 6	1.9300	2.0500	14.8700	7.0400	8.8300	9.9300	1.7900
Region 7	3.2300	4.1100	16.8100	13.3400	10.1200	15.9600	4.3800
Region 8	4.5800	7.6700	18.8300	18.2600	11.4100	16.5700	7.4900
Region 9	6.2300	8.3100	19.0400	20.6200	14.0700	13.2700	11.7500
Region 10	8.5600	12.0200	15.0300	18.2500	12.2800	11.8300	13.1200
Region 11	10.7300	10.1200	6.3000	13.3400	10.9500	10.2800	13.6500
Region 12	11.6900	9.4400	0.3500	6.1000	8.7700	5.5800	12.5700
Region 13	13.5200	6.5100	0.2200	0.4000	5.8600	4.1900	10.7800
Region 14	11.2100	12.6500	0.2000	0.2900	4.3600	2.9400	7.4800
Region 15	12.4100	9.6700	0.1600	0.2000	3.4100	1.6100	6.2700
Region 16	7.8000	9.3700	0.1400	0.1600	2.5000	0.9800	4.5000
Region 17	5.4800	3.6300	0.0600	0.0700	1.0100	0.3100	2.8000
Region 18	0.5700	2.0600	0.0500	0.0500	0.3500	0.0000	1.4900
Region 19	0.1100	0.9100	0.0100	0.0200	0.0400	0.1600	0.6300
Region 20	0.7800	1.0000	0.0500	0.1100	0.2400	0.2400	0.9000

SAMPLE	21889DM1	21891DM1	21957DM1	21966DM1	21999DM1	22059DM1	22441DM1
Region 1	0.0300	0.0000	0.0000	0.0100	0.0200	0.0000	0.0000
Region 2	0.0300	0.0000	0.0200	0.0000	0.0100	0.0000	0.0000
Region 3	0.1500	0.0400	0.1500	0.0100	0.1200	0.0100	0.0200
Region 4	0.2800	0.1900	0.7100	0.1300	0.3300	0.0600	0.1300
Region 5	0.7300	0.9300	4.2100	0.3800	0.6100	0.3700	0.6000
Region 6	2.0100	3.4600	7.5800	1.5800	1.9100	1.4500	2.5500
Region 7	4.7700	7.5000	7.6700	4.0900	4.3000	3.7600	5.3200
Region 8	9.9600	7.8900	8.5600	4.9600	5.9100	4.6600	7.4000
Region 9	9.2900	12.7000	10.5100	10.8200	9.1800	10.0500	11.2000
Region 10	12.8100	13.9400	10.7200	13.6900	14.0600	14.0000	12.9600
Region 11	13.4500	9.6900	10.4700	14.7200	10.8200	14.3800	12.6800
Region 12	10.1300	11.8800	9.7000	13.3500	10.7800	9.5100	11.6800
Region 13	7.5300	9.3300	6.5900	9.8300	11.3000	10.0800	10.6700
Region 14	6.8700	7.8300	5.1200	11.2300	8.7500	7.9000	8.6700
Region 15	7.5100	6.3000	4.3700	6.9700	7.7700	9.9900	6.2900
Region 16	4.6500	4.9600	4.0200	4.5700	6.2800	6.7100	4.0300
Region 17	3.9800	1.9900	3.7700	3.0900	5.4800	5.4000	3.7100
Region 18	2.6000	0.9200	1.8400	0.2600	1.7100	1.7900	1.0800
Region 19	1.4500	0.1000	1.0200	0.0600	0.1300	0.0000	0.0500
Region 20	1.7700	0.3400	2.9500	0.2300	0.4900	0.0000	0.8500

SAMPLE	22461DM1	22479DM1	22492DM1	22503DM1	22555DM1	22558DM1	22607DM2
Region 1	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Region 2	0.0000	0.0000	0.0000	0.0100	0.0000	0.0000	0.0000
Region 3	0.0100	0.0200	0.0200	0.0600	0.0200	0.0000	0.0200
Region 4	0.1100	0.1400	0.1500	0.2600	0.1100	0.0500	0.1400
Region 5	0.6500	0.7700	0.6600	0.9000	0.5500	0.4700	0.6700
Region 6	2.7600	3.5800	2.5700	3.3400	2.3500	2.4400	2.7600
Region 7	5.4200	10.6100	5.8500	8.0500	5.3100	5.0900	8.2400
Region 8	7.2400	15.4200	8.1400	11.5200	7.2300	6.9900	8.3400
Region 9	10.4000	16.1000	11.8100	13.7700	10.7600	11.5400	13.2700
Region 10	13.6000	11.1200	12.2400	11.5700	13.5500	13.7500	14.7300
Region 11	13.7400	10.0000	11.4800	10.3000	13.7800	9.8500	10.8100
Region 12	13.4500	6.4100	10.9300	9.6500	13.0300	14.2500	10.4900
Region 13	12.4200	6.0200	7.4600	7.6100	8.3600	12.7900	10.0700
Region 14	6.7400	4.8700	8.3700	6.0800	9.2400	7.1100	7.7100
Region 15	5.0100	4.0000	7.2600	5.0800	5.2600	5.8500	6.0500
Region 16	3.8600	4.4300	4.7900	4.7700	4.5300	4.6800	4.8600
Region 17	3.1500	3.7500	4.4600	3.9700	3.9600	3.8800	1.3700
Region 18	0.8800	1.2500	1.5600	1.4400	1.1200	0.3200	0.2200
Region 19	0.0700	0.0700	0.0000	0.1000	0.0600	0.0400	0.0600
Region 20	0.5000	1.4400	2.2200	1.5100	0.7800	0.8900	0.1900

SAMPLE	22607DM3	22651DM1	22818DM1	23086DM1	23244DM1		
Region 1	0.0100	0.0000	0.0000	0.0100	0.0000		
Region 2	0.0000	0.0000	0.0000	0.0000	0.0000		
Region 3	0.0300	0.0200	0.0200	0.0100	0.0000		
Region 4	0.1900	0.1300	0.0600	0.0100	0.0100		
Region 5	0.4900	0.9200	0.3200	0.3500	0.2400		
Region 6	2.1200	2.3600	1.7400	1.3900	2.6400		
Region 7	5.8500	6.5400	4.1100	2.3900	11.6000		
Region 8	7.8000	7.3700	7.9900	6.0400	20.5600		
Region 9	11.4000	13.4400	9.9700	10.0200	27.4000		
Region 10	12.9500	15.0100	13.0300	12.3400	18.7500		
Region 11	13.4000	10.4300	14.1200	14.7600	14.5000		
Region 12	12.6900	9.4400	13.1400	11.5000	3.1600		
Region 13	8.9700	8.8800	9.3700	9.7600	0.3600		
Region 14	7.3900	7.2900	8.0300	8.8200	0.2200		
Region 15	6.3900	6.4100	6.7000	6.8000	0.1300		
Region 16	4.9000	5.7000	3.3300	6.3900	0.1100		
Region 17	3.9900	3.0500	5.0000	4.3800	0.1100		
Region 18	0.4600	1.8100	1.6000	2.4600	0.0600		
Region 19	0.1000	0.2000	0.6400	1.3900	0.0000		
Region 20	0.8800	1.0000	0.8200	1.0900	0.1700		

Appendix B

Numerical Formulas For Calculating Predicted
Parameters' Values Using the Percent Peak Area
in Segmented Regions.

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Summer-Hire Prediction Calculations

For the prediction of properties using the model created from the GC traces run by the Summer-hire students the following calculations are performed on the 20 segmented regions. An X-offset value is subtracted from each of the regions to give a corrected X value which is used for the multivariate correlation model. The corrected X value is multiplied by a parameter slope factor and the products are summed to give an uncorrected parameter value. The parameter's predicted value is corrected by adding a Y-offset value.

The following are a listing of the X-offset values and the segmented region multipliers.

CELL #	X-OFFSET	10% BP TEMP. (1×10^{-1})	50% BP TEMP. (1×10^{-1})	90% BP TEMP. (1×10^{-1})	FIN. BP TEMP (1×10^{-1})	DEN (1×10^{-4})	VIS @25°C (1×10^{-3})
1	0.220	-3.541	-2.011	-0.627	-0.429	-0.595	-1.646
2	1.358	-13.42	-9.606	-4.558	-4.194	-3.681	-7.312
3	5.163	-10.77	-12.61	-15.71	-14.06	-11.73	-17.41
4	5.531	-5.033	-10.78	-18.63	-17.64	-12.94	-14.49
5	2.356	-18.17	-13.17	-5.642	-4.855	-4.387	-11.83
6	4.208	-17.26	-12.68	-6.510	-5.713	-4.810	-16.08
7	6.906	-4.042	-6.055	-6.557	-6.230	-3.871	-16.01
8	8.267	0.138	-3.090	-4.835	-4.415	-2.369	-14.14
9	10.59	4.931	1.218	-0.067	-0.163	1.169	-7.412
10	11.30	10.64	7.398	5.509	4.343	4.843	5.446
11	9.957	11.82	9.570	7.948	7.158	5.839	11.53
12	8.467	9.946	10.47	10.37	9.775	7.478	17.41
13	6.968	9.083	10.18	10.09	9.341	6.830	18.17
14	6.058	7.939	8.837	8.994	8.195	6.064	16.92
15	4.779	7.077	7.878	7.445	6.793	4.880	14.35
16	3.638	5.052	6.024	5.772	5.281	3.545	10.71
17	2.546	3.474	4.583	4.245	4.028 .	2.470	7.738
18	0.784	1.116	1.643	1.379	1.335	0.790	2.108
19	0.249	0.191	0.499	0.422	0.435	0.203	0.658
20	0.586	0.829	1.464	1.073	1.113	0.429	14.50

The following is a listing of the Y-offset values which are added to the raw prediction value to give the calculated prediction result.

The following are the Y-offset value for each parameter:

the 10% BP Temperature - 460.138 °K
the 50% BP Temperature - 505.545 °K
the 90% BP Temperature - 555.307 °K
the Final BP Temperature - 585.188 °K
the Density at 25°C - 0.823 Kg/L
the Viscosity at 40°C - 2.235 cSt

Previously-Ran Single Operator Prediction Calculations

For the prediction of properties using the model created from the GC traces run by a single operator the following calculations are performed on the 20 segmented regions. An X-offset value is subtracted from each of the regions to give a corrected X value which is used for the multivariate correlation model. The corrected X value is multiplied by a parameter slope factor and the products are summed to give an uncorrected parameter value. The parameter's predicted value is corrected by adding a Y-offset value.

The following are a listing of the X-offset values and the segmented region multipliers.

CELL #	X-OFFSET	10% BP TEMP. (1×10^{-1})	50% BP TEMP. (1×10^{-1})	90% BP TEMP. (1×10^{-1})	FIN. BP TEMP (1×10^{-1})
1	2.632	-12.39	-28.79	-42.36	-54.98
2	5.338	-20.82	-20.70	-4.465	0.144
3	10.60	-15.38	-9.155	-5.305	1.095
4	11.76	2.516	-6.949	-18.99	-22.61
5	6.900	-5.030	-7.433	-12.25	-11.03
6	9.078	-7.161	-3.012	16.75	15.57
7	11.13	3.829	0.126	-6.528	-9.489
8	11.31	5.669	1.652	-6.590	-5.211
9	10.43	3.883	3.792	1.337	6.105
10	7.600	7.396	1.078	1.760	0.434
11	5.130	10.10	6.391	7.642	-0.674
12	2.610	7.153	7.004	6.507	2.402
13	1.648	7.179	13.03	14.65	17.91
14	1.189	5.914	14.41	17.13	21.96
15	0.884	5.231	10.36	10.30	12.47
16	0.782	4.852	9.600	10.13	12.14
17	0.462	2.992	5.811	7.135	8.617
18	0.241	0.992	2.559	2.285	2.938
19	0.112	0.537	1.723	2.227	2.952
20	0.212	-0.411	-0.821	-0.230	0.726

CELL #	X-OFFSET	DEN. $(1x10^{-4})$	VIS. $(1x10^{-3})$
1	2.389	-14.62	-19.69
2	4.948	-14.97	-29.73
3	9.816	-9.141	-21.05
4	10.81	-10.14	-1.325
5	6.792	6.444	-10.84
6	9.246	-2.900	-7.371
7	11.51	1.334	-1.740
8	11.70	0.139	-10.19
9	10.87	0.474	-2.906
10	7.906	-0.288	0.523
11	5.269	4.454	13.51
12	2.636	5.997	13.43
13	1.720	9.300	20.17
14	1.230	8.903	19.60
15	0.941	7.526	16.88
16	0.902	4.453	10.25
17	0.556	2.208	5.310
18	0.314	0.059	1.230
19	0.170	0.259	0.275
20	0.241	0.884	4.262

The following is a listing of the Y-offset values which are added to the raw prediction value to give the calculated prediction result.

The following are the Y-offset value for each parameter:

the 10% BP Temperature - 130.782 °K
the 50% BP Temperature - 172.565 °K
the 90% BP Temperature - 215.053 °K
the Final BP Temperature - 245.963 °K
the Density at 25°C - 0.781 Kg/L
the Viscosity at 40°C - 1.473 cSt

Prediction Calculations Using Data From The Summer-Hire Students and the Previously-Ran Single Operator Data

For the prediction of properties using the model created from the GC traces run by a single operator and combined with data from GC runs performed by the summer-hire students, the following calculations are performed on the 20 segmented regions. An X-offset value is subtracted from each of the regions to give a corrected X value which is used for the multivariate correlation model. The corrected X value is multiplied by a parameter slope factor and the products are summed to give an uncorrected parameter value. The parameter's predicted value is corrected by adding a Y-offset value.

The following are a listing of the X-offset values and the segmented region multipliers.

CELL #	X-OFFSET	10% BP TEMP. (1×10^{-1})	50% BP TEMP. (1×10^{-1})	90% BP TEMP. (1×10^{-1})	FIN. BP TEMP (1×10^{-1})
1	2.242	-4.965	-29.52	-41.86	-55.06
2	4.677	-12.12	-19.88	-3.401	7.250
3	9.713	-14.41	-8.912	-6.257	-2.274
4	10.08	-3.489	-7.692	-19.75	-22.67
5	5.991	-16.13	-7.124	-10.71	-13.33
6	8.339	-10.64	±4.198	14.33	16.11
7	10.82	-2.701	0.874	-5.908	-7.548
8	11.29	1.318	0.726	-8.595	-8.346
9	10.82	4.311	2.210	1.999	4.894
10	8.313	8.434	3.523	2.804	0.570
11	5.827	9.920	5.851	7.322	-1.053
12	3.306	9.601	6.634	6.334	2.387
13	2.259	8.549	12.98	14.47	17.59
14	1.735	7.501	14.72	16.82	21.00
15	1.341	5.787	11.57	11.57	13.13
16	1.112	4.571	10.07	10.60	12.13
17	0.711	3.015	6.909	8.401	10.47
18	0.295	1.024	2.205	2.017	2.898
19	0.118	0.471	1.058	1.178	1.962
20	0.246	0.312	-1.372	-0.820	-0.044

CELL #	X-OFFSET	DEN. (1×10^{-4})	VIS. (1×10^{-3})
1	2.143	-10.35	-18.49
2	4.542	-12.76	-28.10
3	9.290	-13.08	-22.01
4	10.21	-8.767	-3.033
5	6.290	6.210	-9.061
6	8.676	-4.146	-7.361
7	10.99	-1.532	-2.113
8	11.31	-1.252	-10.72
9	10.84	1.468	-4.406
10	8.291	3.3878	0.476
11	5.799	5.789	12.57
12	3.296	7.121	13.41
13	2.314	7.861	20.23
14	1.838	7.202	19.61
15	1.375	6.046	17.67
16	1.211	3.751	10.69
17	0.782	2.287	6.077
18	0.367	0.321	1.182
19	0.179	0.085	0.068
20	0.280	0.563	4.018

The following is a listing of the Y-offset values which are added to the raw prediction value to give the calculated prediction result.

The following are the Y-offset value for each parameter:

the 10% BP Temperature - 417.681 °K
the 50% BP Temperature - 454.390 °K
the 90% BP Temperature - 497.298 °K
the Final BP Temperature - 528.854 °K
the Density at 25°C - 0.786 Kg/L
the Viscosity at 40°C - 1.560 cSt

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APPENDIX C

Plots of measured Versus Predicted Parameters using Models Generated Using Data from GC Traces of the Summer-Hire Students Combined with Previously-Ran Single Operator Data

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10% BP TEMP. (12 MINUTE ANALYSIS)
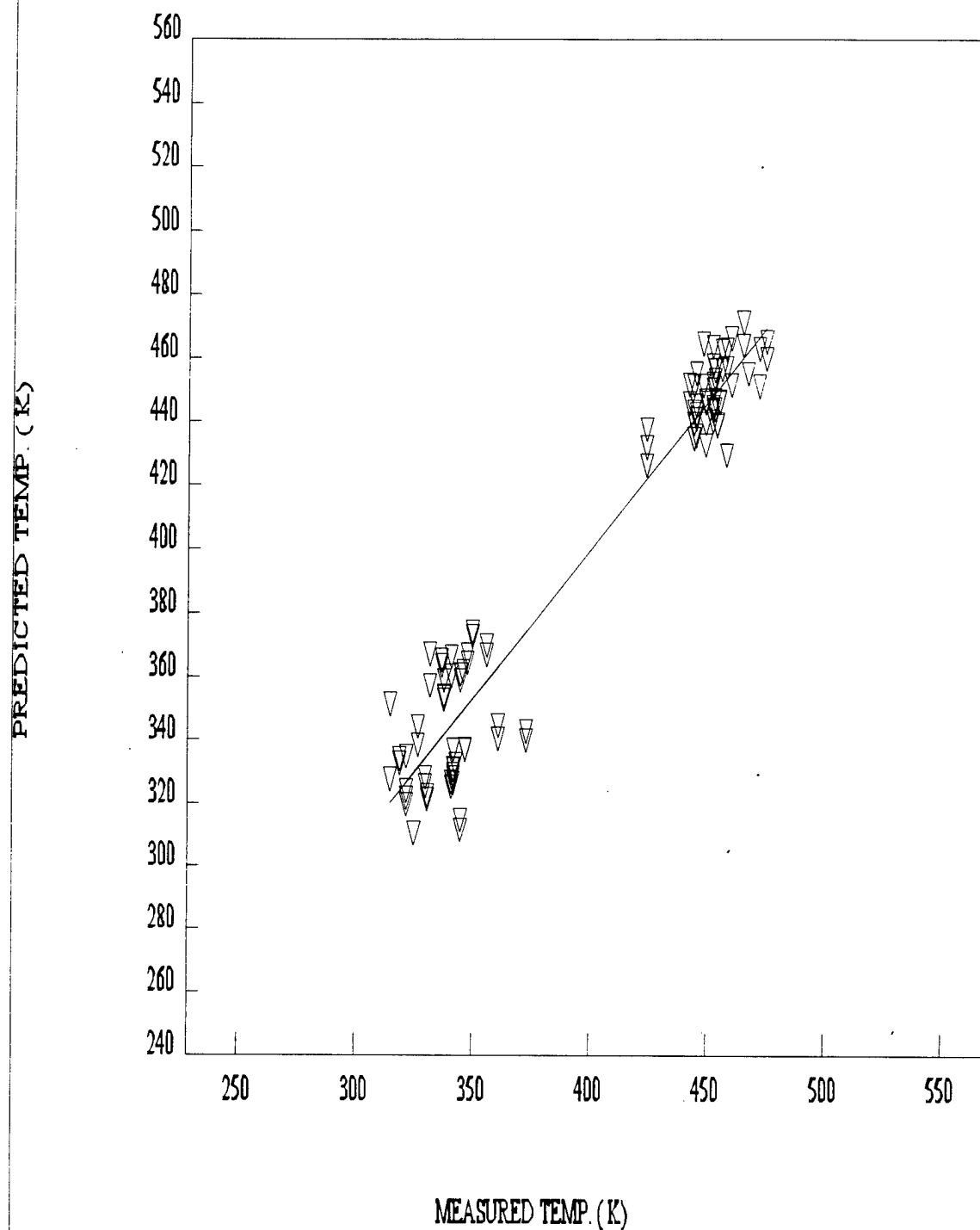
RSQUARED=0.9354

50% BP TEMP. (12 MINUTE ANALYSIS)
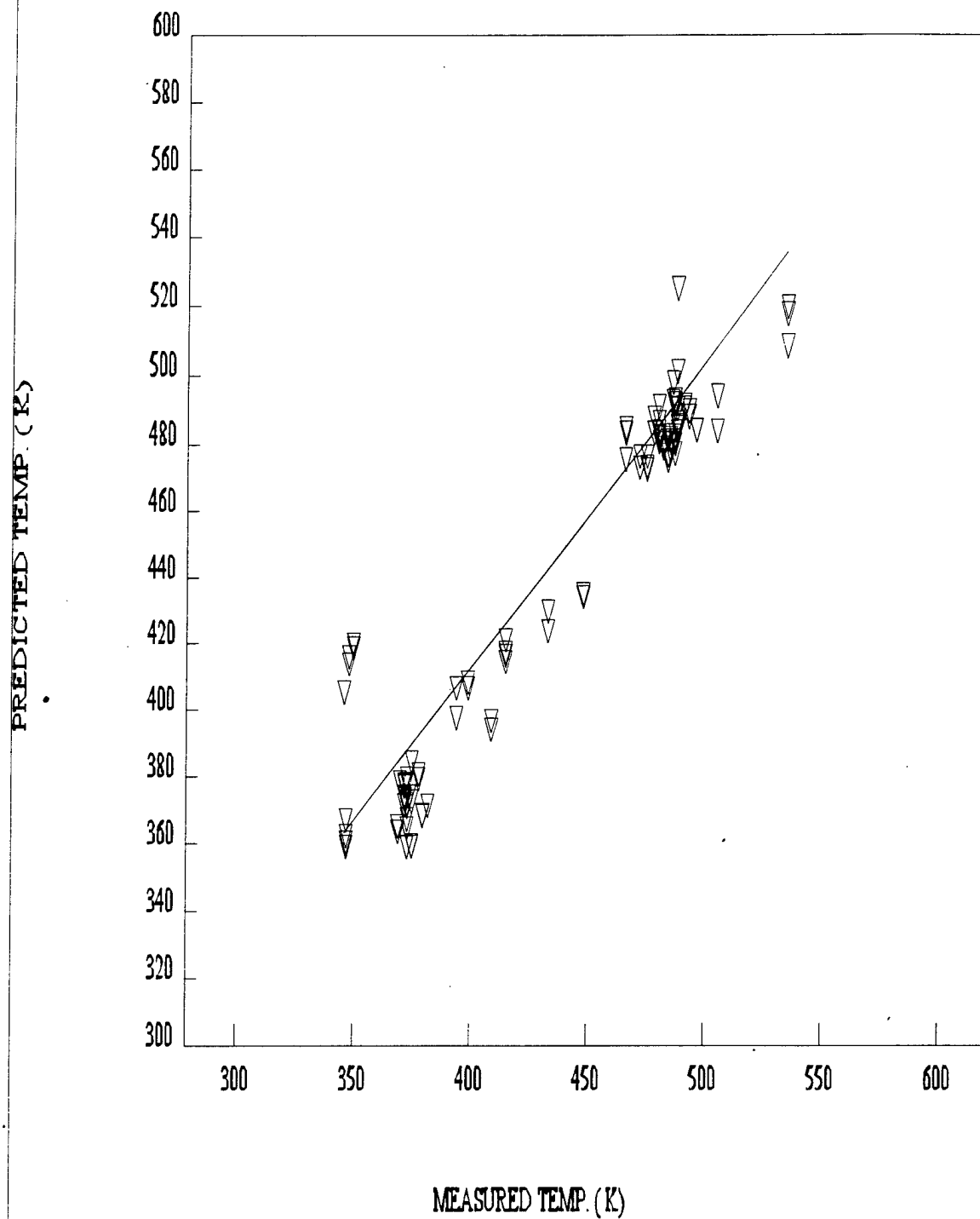
RSQUARED=0.9143

90% BP TEMP. (12 MINUTE ANALYSIS)
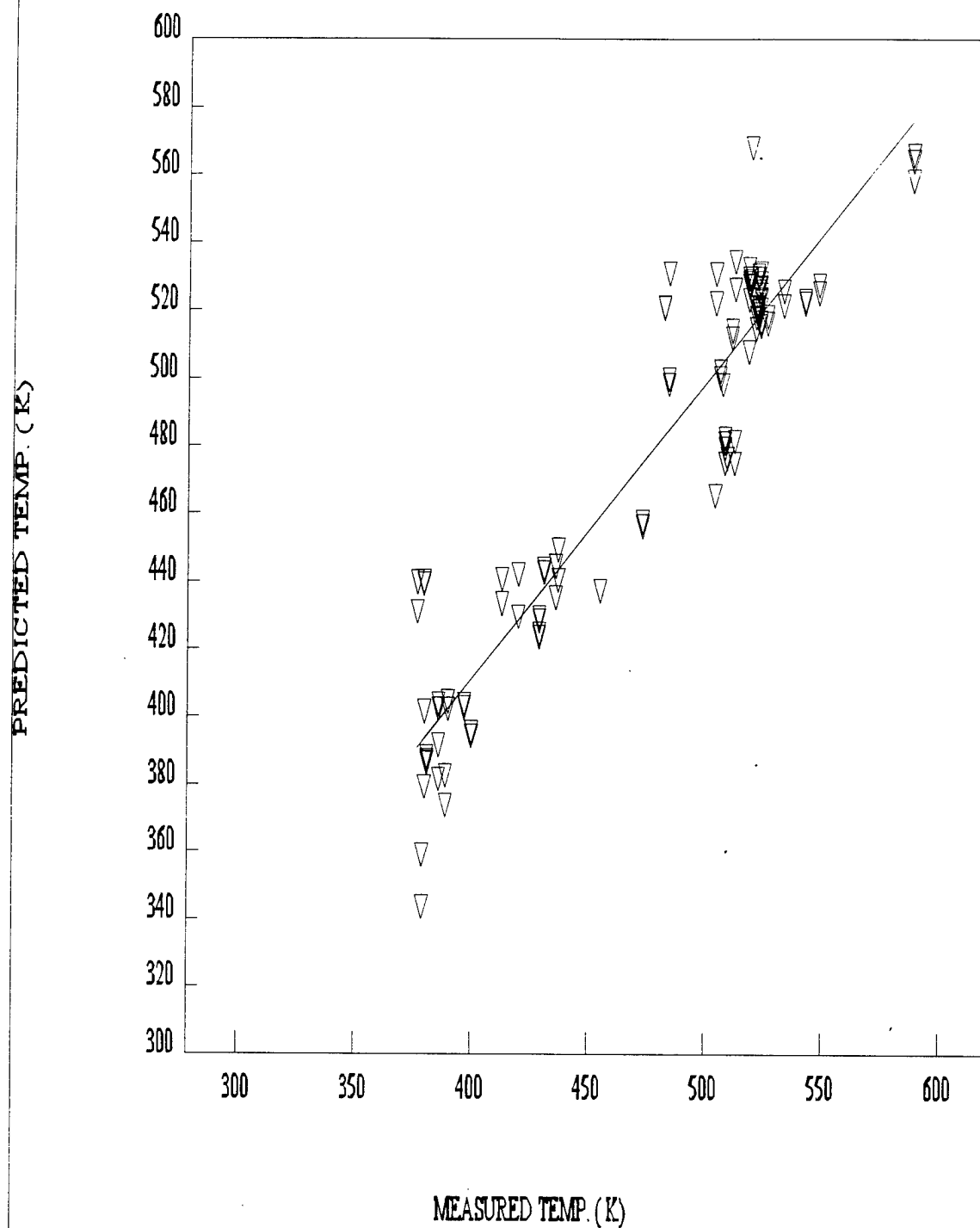
RSQUARED=0.8827
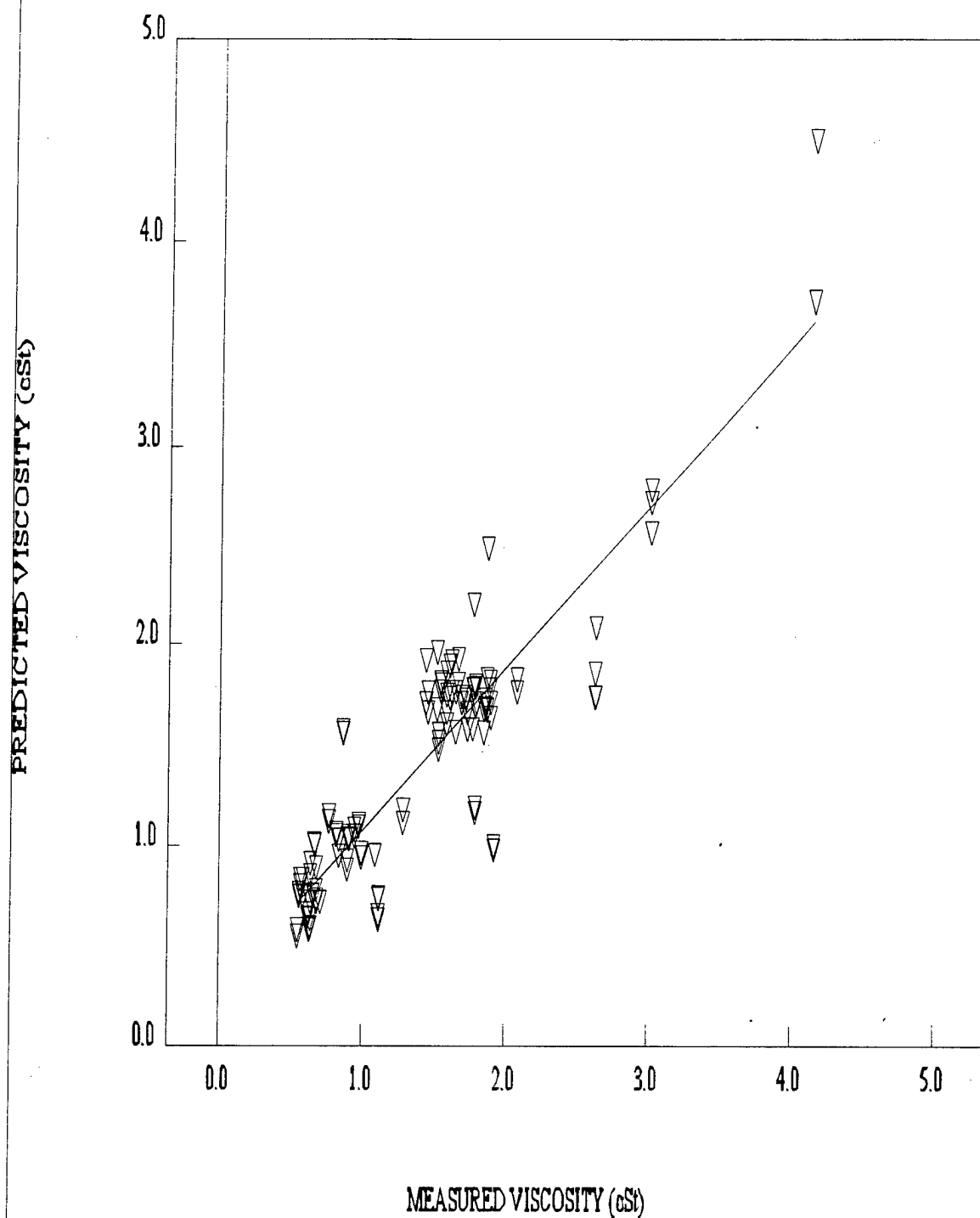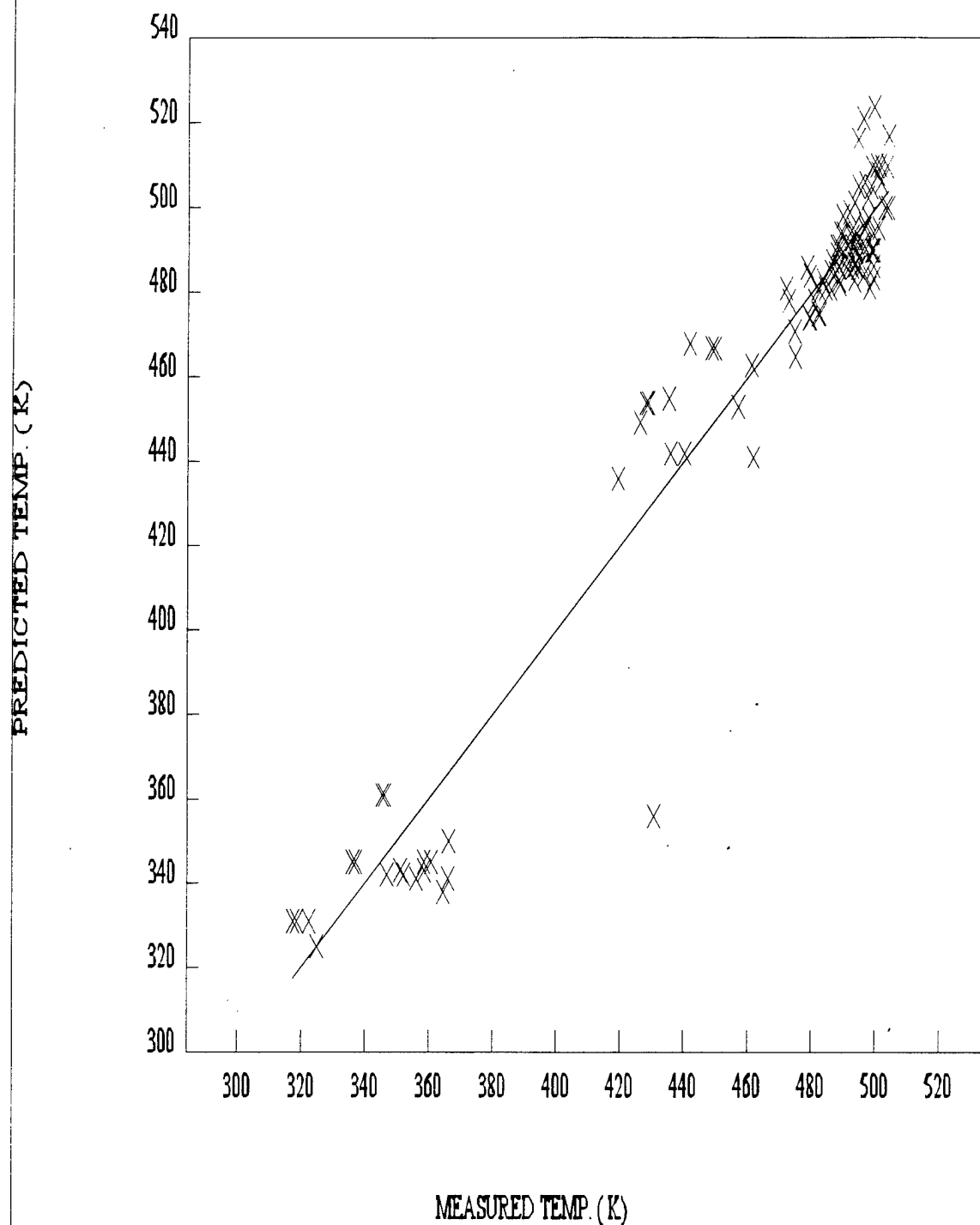
FINAL BP TEMP. (12 MINUTE ANALYSIS)
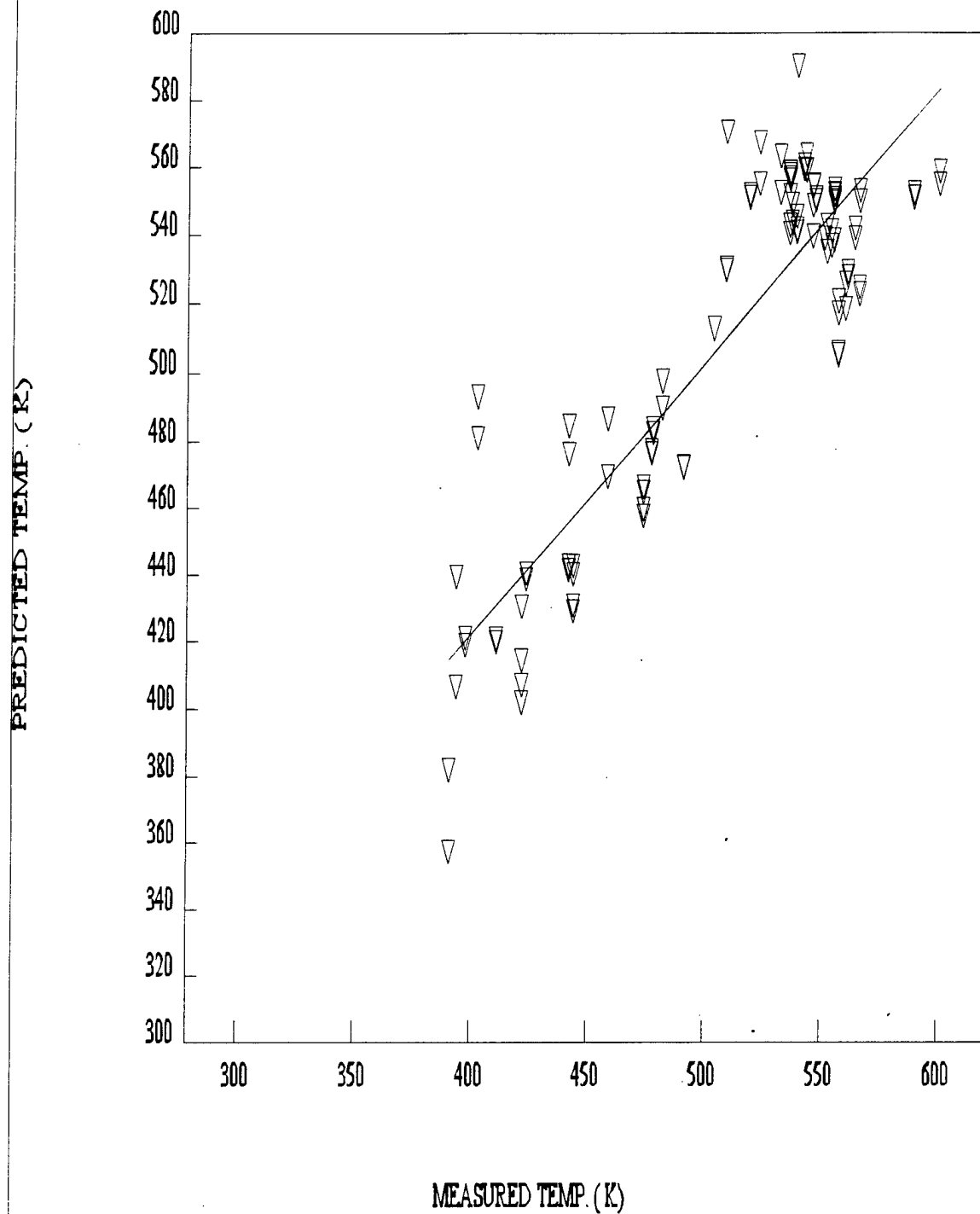
RSQUARED=0.8014

DENSITY (12 MINUTE ANALYSIS)
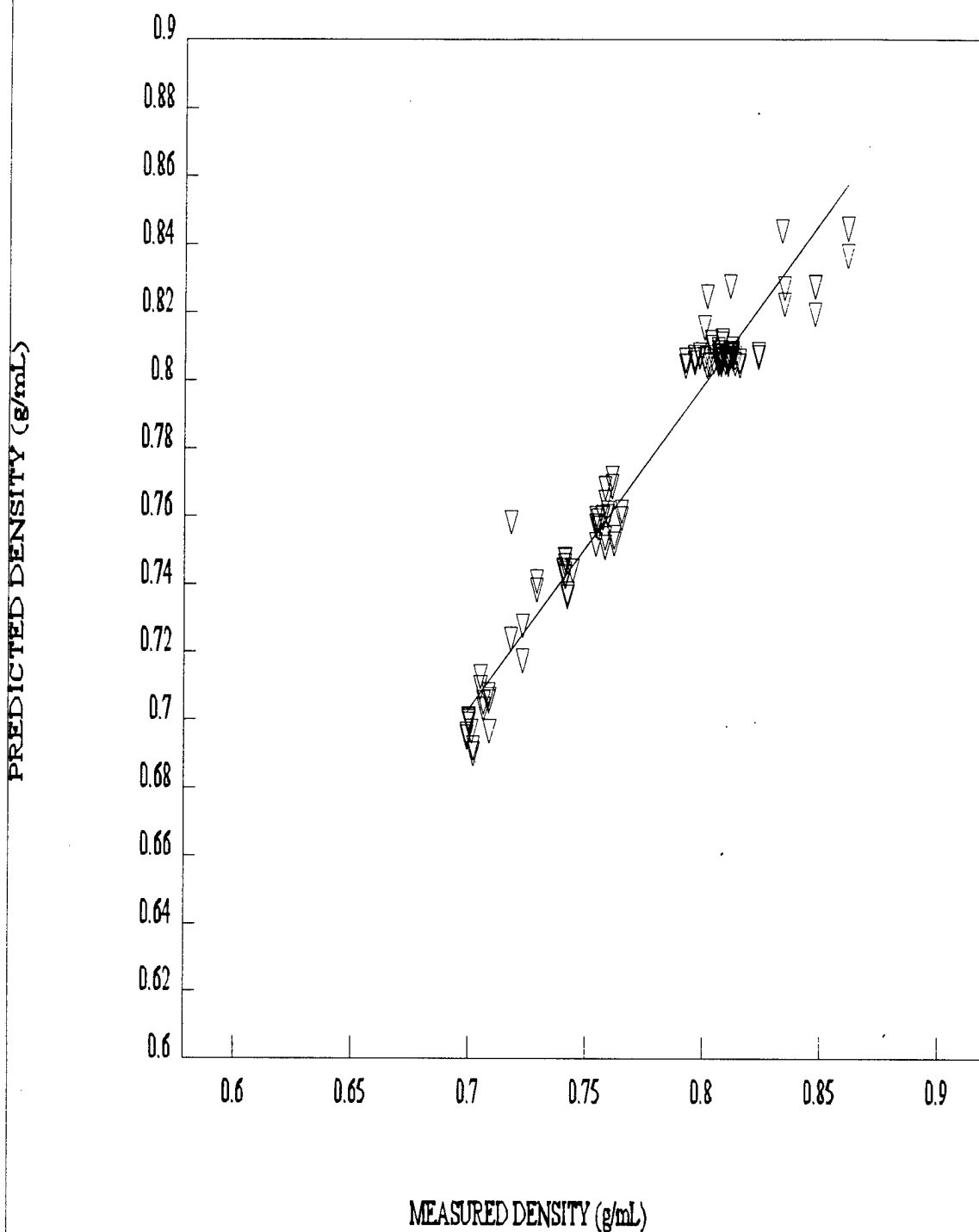
RSQUARED=0.9602

VISCOSITY @ 40 C (12 MINUTE ANALYSIS)
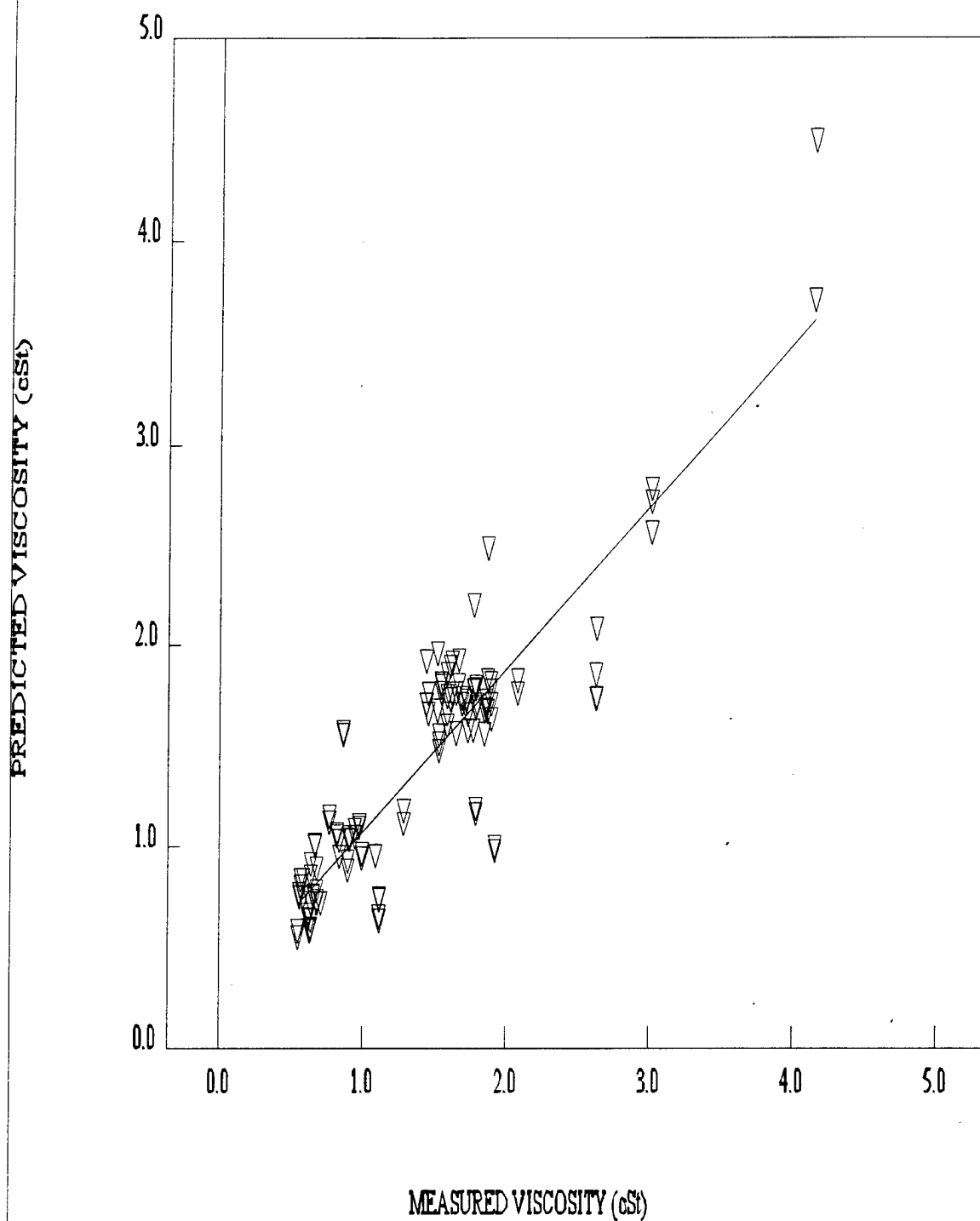
RSQUARED=0.8083

APPENDIX D

Plots of measured Versus Predicted Parameters using Models Generated Using Data from GC Traces of the Summer-Hire Students
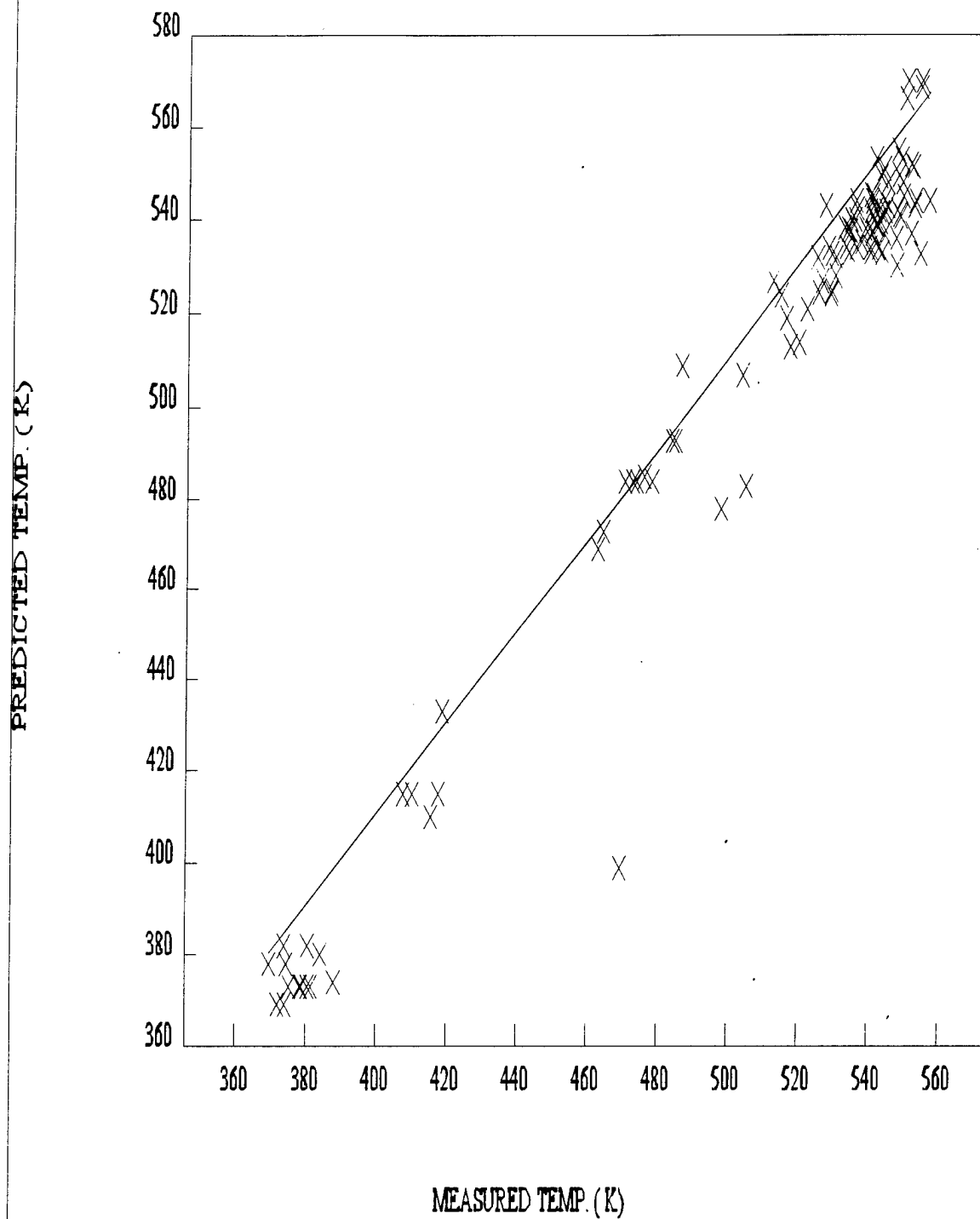
(intentionally left blank)

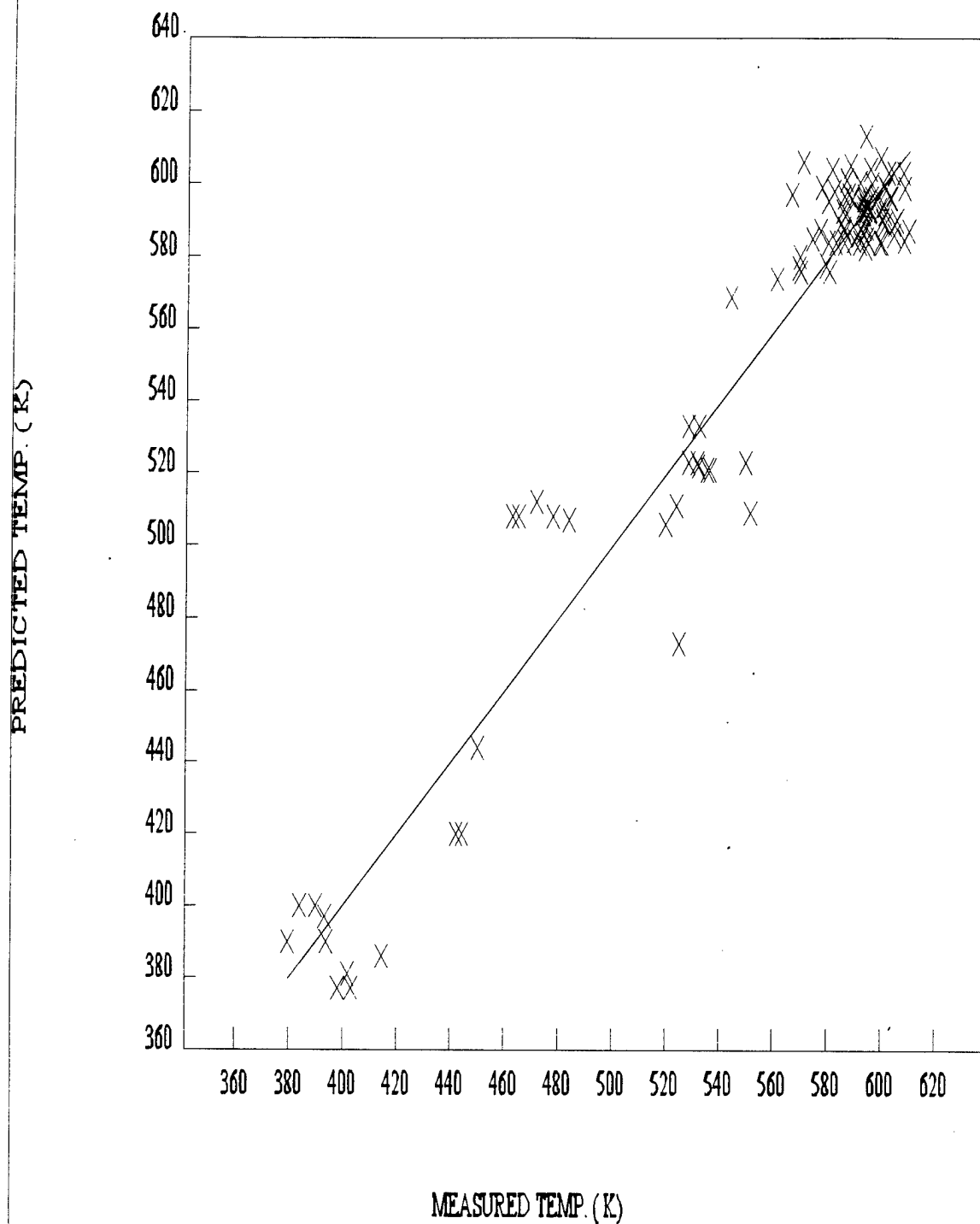# 10% BP TEMP. (12 MINUTE ANALYSIS)

RSQUARED=0.9354

PREDICTED TEMP. (K)

MEASURED TEMP. (K)

50% BP TEMP. (12 MINUTE ANALYSIS)

RSQUARED=0.9143

MEASURED TEMP. (K)

90% BP TEMP. (12 MINUTE ANALYSIS)

RSQUARED=0.8827

FINAL BP TEMP. (12 MINUTE ANALYSIS)

RSQUARED=0.8014

PREDICTED TEMP. (K)

MEASURED TEMP. (K)
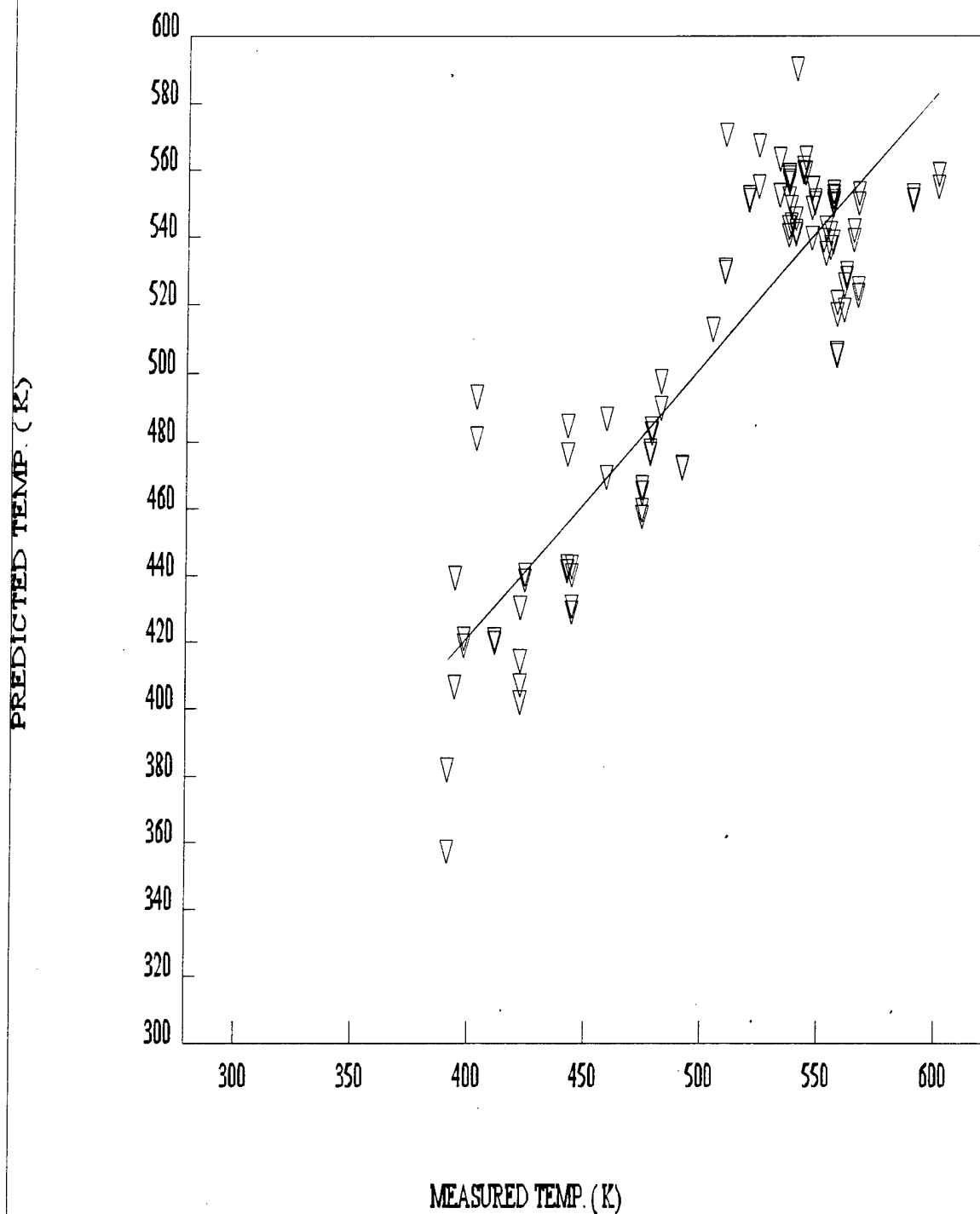
DENSITY (12 MINUTE ANALYSIS)

RSQUARED=0.9602

VISCOSITY @ 40 C (12 MINUTE ANALYSIS)

RSQUARED=0.8083

APPENDIX E

Plots of measured Versus Predicted Parameters using Models Generated Using Data from GC Traces of the Summer-Hire Students

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10% BP TEMP

R SQUARED = 0.9474

PREDICTED TEMP. (K)

MEASURED TEMP. (K)

50% BP TEMP

R SQUARED = 0.9678

90% BP TEMP

R SQUARED = 0.9425

PREDICTED TEMP. (K)

MEASURED TEMP. (K)

FINAL BP TEMP

R SQUARED = 0.8651

PREDICTED TEMP. (K)

MEASURED TEMP. (K)
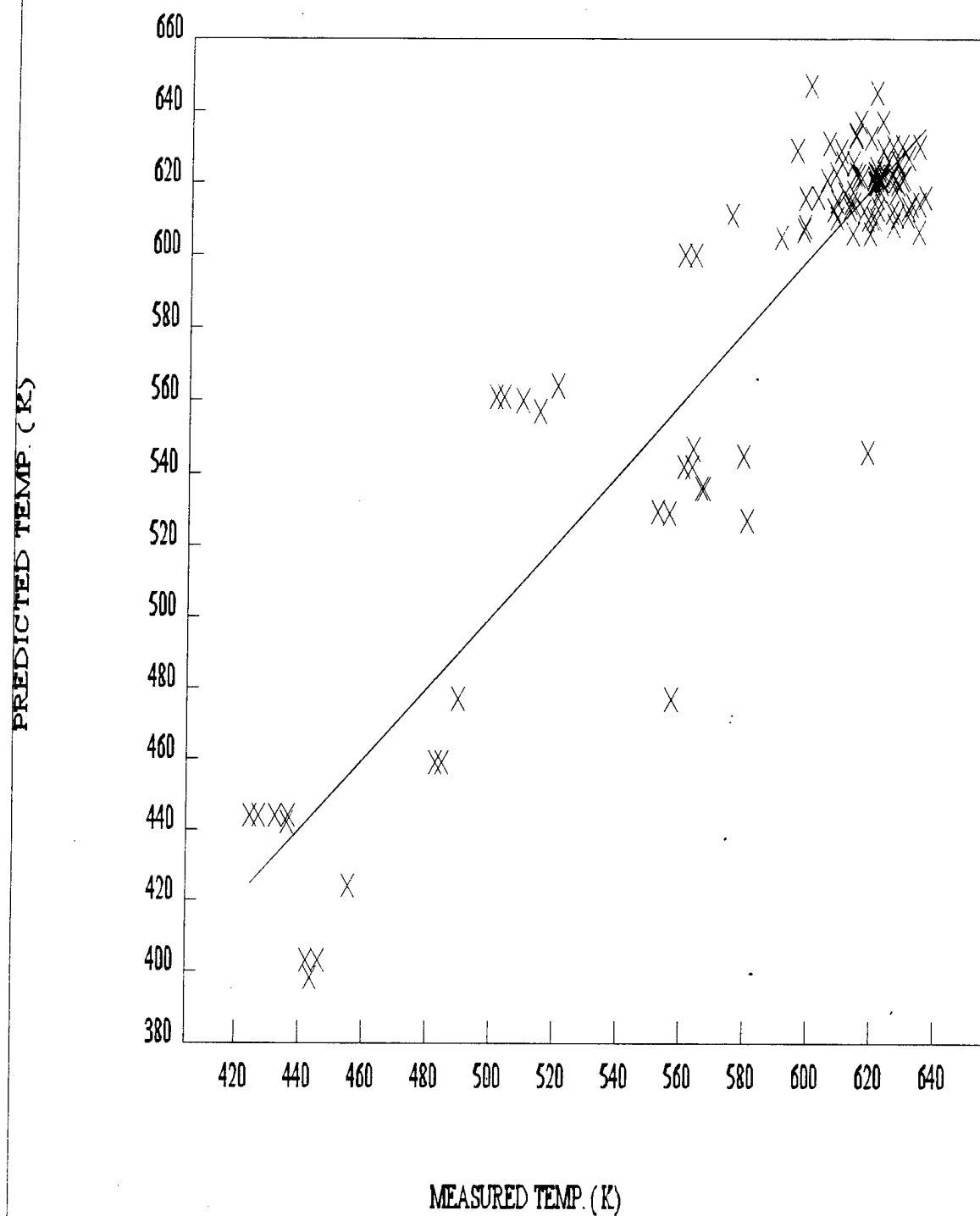
DENSITY @ 25 C

R SQUARED = 0.9601

PREDICTED DENSITY (Kg/L)

MEASURED DENSITY (Kg/L)
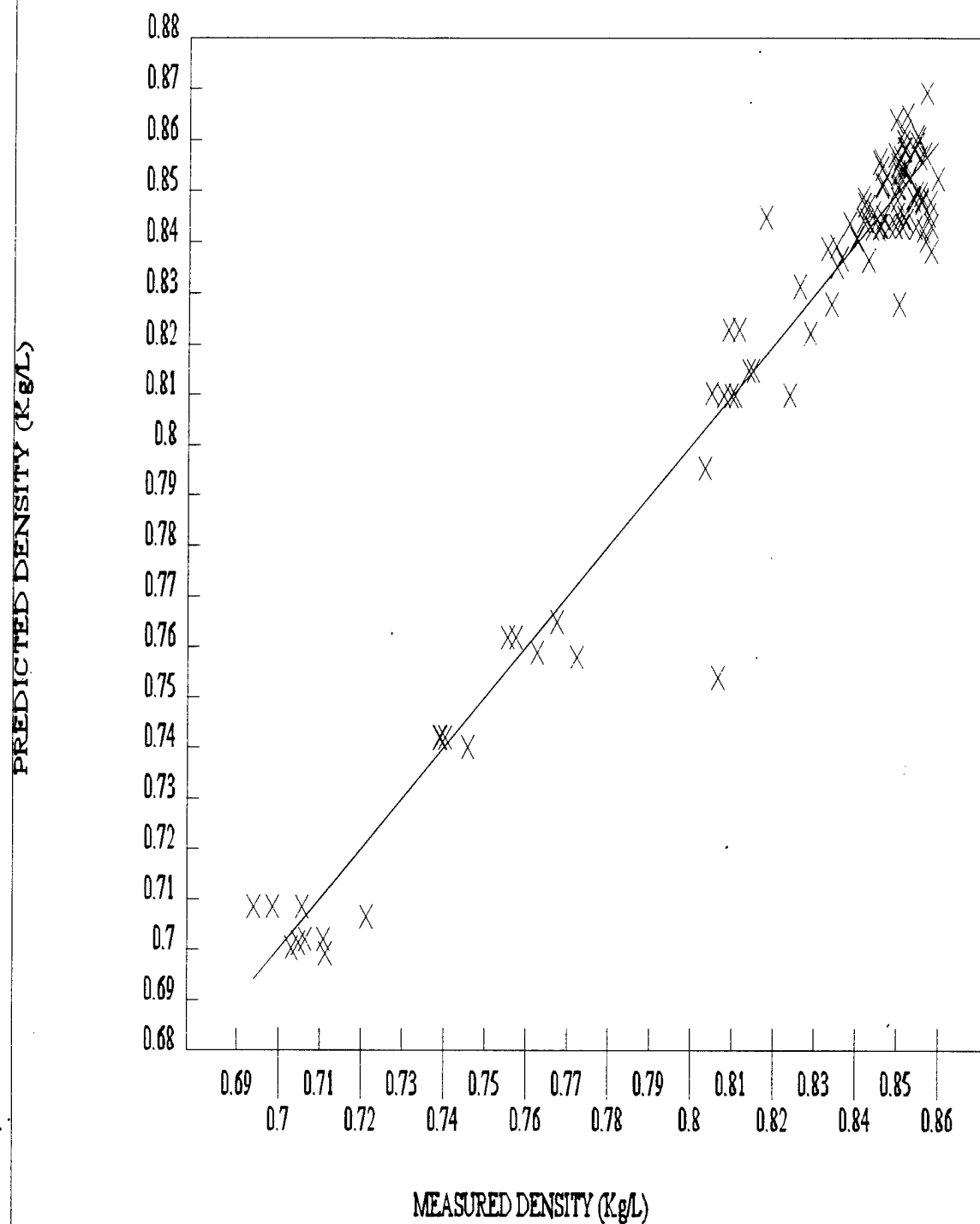
VISCOSITY @ 40 C

R SQUARED = 0.8990

PREDICTED VISCOSITY (cSt)

MEASURED VISCOSITY (cSt)
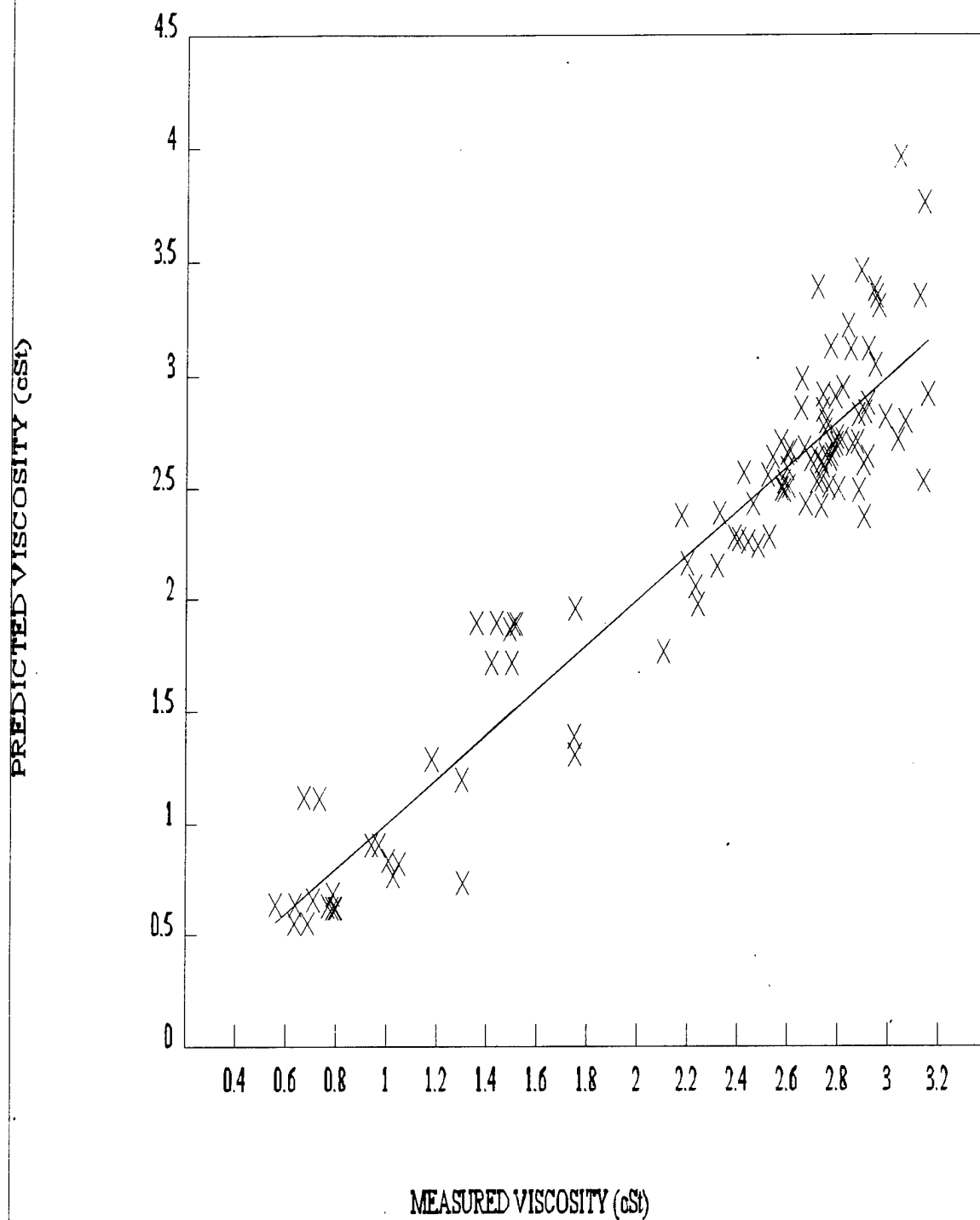
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1 ATTN DALO TSE
1 ATTN DALO SM
    500 PENTAGON
    WASHINGTON DC 20310-0500

    SARDA
1 ATTN SARD TT
    PENTAGON
    WASHINGTON DC 20310-0103

    CDR AMC
1 ATTN AMCRD S
1 ATTN AMCRD IT
    5001 EISENHOWER AVE
    ALEXANDRIA VA 22333-0001

    CDR ARMY TACOM
1 ATTN AMSTA TR NAC
1 ATTN AMSTA TR R/121
1 ATTN AMSTA IM H
    WARREN MI 48397-5000

    MOBILITY TECH CTR BELVOIR
10 ATTN AMSTA RBW
 1 ATTN AMSTA RBXA
    10115 GRIDLEY RD STE 128
    FT BELVOIR VA 22060-5843

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    ARMY RSCH LAB
1 ATTN AMSRL CP PW
    2800 POWDER MILL RD
    ADELPHIA MD 20783-1145

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    NASA LEWIS RSCH CTR
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    CDR AMSAA
1 ATTN AMXSY CM
1 ATTN AMXSY L
    APG MD 21005-5071

CDR ARO
1 ATTN AMXRO EN(D MANN)
   RSCH TRIANGLE PK
   NC 27709-2211

CDR ARMY NRDEC
1 ATTN SATNC US (J SIEGEL)
1 ATTN SATNC UE
   NATICK MA 01760-5018

CDR ARMY CRDEC
1 ATTN SMCCR RS
   APG MD 21010-5423

CDR APC
1 ATTN SATPC L
1 ATTN SATPC QE(BLDG 85 3)
   NEW CUMBERLAND
   PA 17070-5005

CDR ARMY TECOM
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1 ATTN AMSTE EQ
   APG MD 21005-5006

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1 ATTN ATCD SL 5
   INGALLS RD BLDG 163
   FT MONROE VA 23651-5194

CDR ARMY QM SCHOOL
1 ATTN ATSM PWD
   FT LEE VA 23001-5000

CDR ARMY SAFETY CTR
1 ATTN CSSC PMG
1 ATTN CSSC SPS
   FT RUCKER AL 36362-5363

CDR ARMY YPG
1 ATTN STEYP MT TL M
   YUMA AZ 85365-9130

CDR ARMY CERL
1 ATTN CECER EN
   P O BOX 9005
   CHAMPAIGN IL 61826-9005

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   2531 JEFFERSON DAVIS HWY
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1 ATTN CODE 632
1 ATTN CODE 859
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   P O BOX 7176
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QUANTICO VA 22134-5080

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MARINE CORPS SYS CMD
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MARINE CORPS SYS CMD
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1   ATTN SSE
2030 BARNETT AVE STE 315
QUANTICO VA 22134-5010

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8725 JOHN J KINGMAN RD
SUITE 2941
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1 ATTN WL/POSF
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NASA
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CLEVELAND OH 44135

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